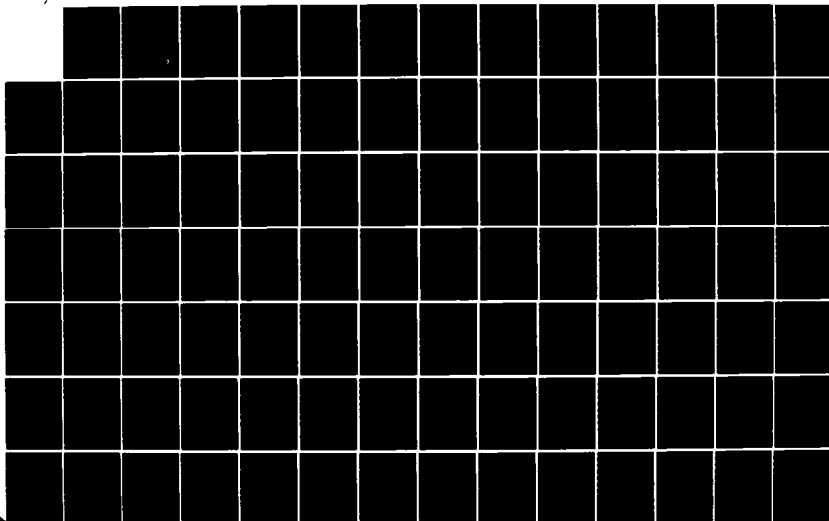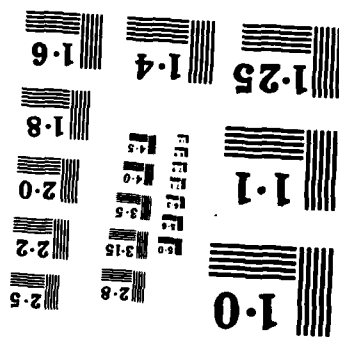AD-A152 192   SIMULATION OF METAL FATE AND TRANSPORT IN THE NAUGATUCK   1/2
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Streifert, Scott Edward (M.S., Civil Engineering)

Simulation of Metal Fate and Transport in the Naugatuck

River (Connecticut) with MEXAMS

Thesis directed by Dr. Allen J. Medine

Metal transport in the Naugatuck River is currently being investigated to provide important data for waste allocation decisions. The development of suitable metals modeling capability is a necessary part of the management activities. The calibration, testing and evaluation of MEXAMS (Metal Exposure Analysis Modeling System) computer program was performed to meet the above requirement.

Results indicate that the log $K_d$ and percent groundwater flow into the benthic compartments value were the most sensitive and were used as the major calibration variables. The model very accurately predicted both the particulate concentration of all benthic compartments and the total and aqueous concentration for all water water column compartments. Now that the initial calibration has been achieved, the verification procedure will be performed and the initial calibration will be fine tuned.
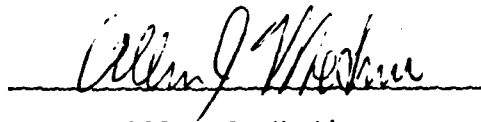
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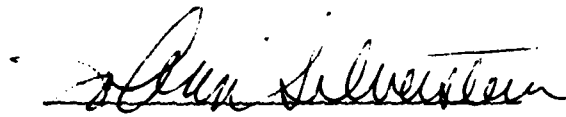
SIMULATION OF METAL FATE AND TRANSPORT

IN THE

NAUGATUCK RIVER (CONNECTICUT) WITH MEXAMS

by

Scott Edward Streifert

B.S.C.E., Norwich University, 1980

A thesis submitted to the

Faculty of the Graduate School of the

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by

_____

Allen J. Medine

_____

JoAnn Silverstein

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DEDICATION

This is dedicated to my parents, Jack and Jane. Their love, support and encouragement during all of my endeavors have been invaluable.

## ACKNOWLEDGEMENTS

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# CHAPTER 1

## INTRODUCTION

### 1.1 General

Heavy metals in our aquatic environments, their transport processes, environmental distributions and biological effects have been the focus of increasing concern. Direct toxicity to aquatic organisms and indirect toxicity to higher organisms and man are the center of this concern. Although heavy metals are natural constituents of aquatic environments, additional quantities introduced by man's presence may result in an altered chemical composition of the aqueous and sediment phases, often with detrimental impacts on the environment. In an effort to reduce these impacts, environmental transport/fate models of heavy metals in aquatic ecosystems are being developed.

The purpose of this study was to evaluate the Metal Exposure Assessment Modeling System (MEXAMS). This program is the result of linking MINTEQ, a geochemical model, and the Aquatic Exposure Assessment Model, EXAMS. MEXAMS was developed for the Environmental Protection Agency (EPA) (Felmy et al., 1983) to allow assessment of

the impacts of priority pollutant metals (As, Cd, Cu, Pb, Ni, Ag and Zn). The evaluation consisted of calibrating, testing, and assessing the model response for actual site application on the Naugatuck River located in the Housatonic River Basin in western Connecticut.

## 1.2 Background Information

The Naugatuck River is located in western Connecticut and has a long history of industrialization along its length. Hydropower generation was responsible for the initial development of the valley, with light metal production soon to follow. Three of the world's largest brass firms were located on its banks and, at the turn of the century, sixty percent of the world's brass products produced annually were manufactured in the valley. As a result of the light metal production industry, the electroplating industry emerged, and approximately 30,300 cubic meters/day of treated electroplating waste is currently being discharged into the Naugatuck River.

Most industrial discharges on the river currently adhere to Best Available Technology (BAT) guidelines. However, both long-term biological monitoring and recent toxicity testing have shown toxic impacts of metals. As a result, the Connecticut Department of Environmental Protection is presently developing allocation guidelines for the discharge of metals into the river. These

guidelines will be based upon results of mathematical modeling being performed by the State Department of Environmental Protection. The data set available was used herein to calibrate MEXAMS to the Naugatuck River and the output will provide a direct comparison of two model formulations for predicting fate and transport of heavy metals in a riverine ecosystem.

# CHAPTER 2

## MODEL DESCRIPTIONS

### 2.1 EXAMS General Description

The Exposure Assessment Model System (EXAMS) was
developed in response to a need to describe fate,
transport and impacts of organic contaminants in aquatic
systems. The program is a deterministic, predictive
systems model, based on a core of mechanistic process
equations derived from fundamental theoretical concepts
(Burns et al., 1981).

The model estimates exposure, fate, and persis-
tence following a priority pollutant metal discharge.
Exposure is defined as the steady-state pollutant con-
centration after loadings are balanced with transport and
transformation processes. Fate is defined as the dis-
tribution of the pollutant in the system, and persistence
is the time required for effective purification of the
system. The program uses conservation of mass to balance
loadings, transport and transformation of the compound.

The chemical loadings can be entered into EXAMS
by way of :

1., Point Source Loadings

2.) Non-Point Source Loadings
3.) Aerial Drift
4.) Atmospheric Washout
5.) Groundwater Seepage

These chemicals can then be transformed by photolysis, hydrolysis, biochemical and oxidation reactions in particular compartments of the environment under simulation. In addition to the above transformation processes, EXAMS is capable of three transport processes: advection (dependent on the hydrologic data input), dispersion (dependent on the description of each dispersive pathway) and volatilization (the air/water interface). Advective and dispersive transport are possible for dissolved species, sediment sorbed material and bio-sorbed materials. Transport through the ecosystem compartments may be represented by whole sediment bed loads, suspended sediment washloads, exchanges with fixed volume sediment beds and ground water infiltration.

EXAMS can also be used to simulate the ionization and sorption of up to fifteen molecular species of an organic chemical. The chemical can be the parent un-charged, singly or doubly charged cations and anions, each of which can occur in the dissolved, sediment-sorbed or bio-sorbed forms. However, EXAMS, like all models, contains important assumptions. These assumptions are listed as follows:

1.) A first order evaluation can be executed

COMPARTMENTALIZATION EXAMPLES

LOTIC SYSTEM

E - EPILIMNION
B - BENTHIC

LENTIC SYSTEM

POSSIBLE PATHWAYS

L - LITTORAL
E - EPILIMNION
H - HYPOLIMNION
B - BENTHIC
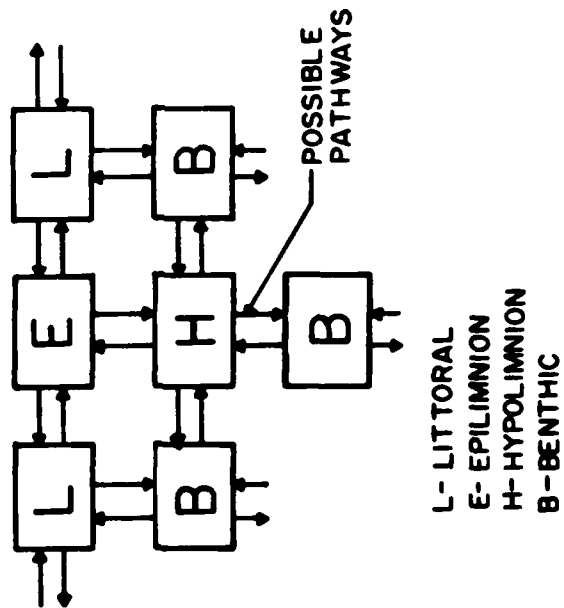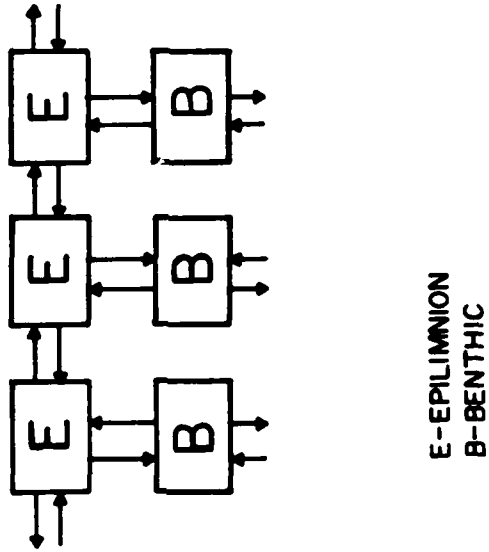
Figure 1.

          independently of the chemicals actual effects
          on the system,

2.) Linear sorption isotherms and second order
expressions are used, rather than Michaelis-
Menten-Monod expressions, for biolysis,

3.) EXAMS was developed for long-term or steady-
state loadings rather than dynamic transitory
(spills) loadings, and

4., Sorption is treated as an equilibrium
process, that is, sorption/desorption are
assumed to be rapid compared to other
processes.

EXAMS is capable of simulating both lotic and
lentic aquatic systems. These systems are initially
compartmentalized and classified as littoral, epilimnion,
hypolimnion or benthic (Figure 1 illustrates compartmen-
talization of a lake system and a river system). Each
compartment is assumed to be completely mixed. The com-
puter then develops single differential equations for
each compartment. The form of the equation and the vari-
ables are defined as:

$$V\left(\frac{dc}{dt}\right) = L_e + L_i - VKC \qquad (1)$$

where:
$V$ = volume of water in compartment (1)
$C$ = total chemical concentration in compartment (mg/l)
$L_e$ = total external loading (mg hr)
$L_i$ = total internal loading (mg hr)
$K$ = overall pseudo-first order loss constant (/hr)
$t$ = time

EXAMS was not originally designed to describe

metal transport and fate and has been modified so that it
can interface with MINTEQ. The first modification in-
volved bypassing calculations that are unnecessary for
heavy metal speciation or duplicated by MINTEQ. The
second modification included provisions for describing
migration and fate of precipitated fractions. Ionization
is not utilized in EXAMS, because MINTEQ calculates
dissolved species in each compartment. Finally, priority
metals are generally unaffected by the transformation and
degradation processes that effect the fate of organics in
natural waters and these processes are bypassed in the
modified EXAMS version.

## 2.2 MINTEQ General Description

MINTEQ is a computer program for calculating
aqueous geochemical equilibria and was developed for
incorporation into MEXAMS. The major objective of MINTEQ
is the development of a predictive methodology for the
assessment of the metal speciation including sorption,
precipitation and ion exchange of priority pollutant
metals in aquatic environments. This chemical equilibrium
problem is described as a set of mass balance equations,
one for each component, and a set of mass action equa-
tions, one for each specie. The equilibrium constant
approach is utilized to solve the equilibrium problem.
This method solves nonlinear mass action expressions

using linear mass balance equations. The typical mass action and mass balance equations are as follows:

### Mass Action:

$$\gamma_i C_i = K_i \sum_{j=1}^{n} X_j \, a(i,j) \tag{2}$$

where:

$\gamma_i$ = activity coefficient of species i
$C_i$ = concentration of species i
$K_i$ = equilibrium constant reaction i
$X_j$ = activity of component j
$a(i,j)$ = stoichiometric coefficient of components in species i
$n$ = number of components

### Mass Balance:

$$T_j = \sum_{j=1}^{m} a(i,j) \, C_i \tag{3}$$

where:

$T_j$ = total analytical concentration of component j
$m$ = number of aqueous species

Both of the above equations are definitions for systems with no solid phases. Solid phases are dealt with using the "transformation of basis" method (Felmy et al., 1983). This method reduces the number of independent variables to be determined and allows the solution of a wider range of chemical equilibrium problems.

MINTEQ is also capable of modeling adsorption in

a number of ways. Six different algorithms are accessible

through the use of MINTEQ for describing sorption

phenomena:

1.) "activity" $K_d$
2.) "activity" Langmiur equation
3.) "activity" Freundlich equation
4.) ion exchange
5.) constant capacitance surface
     complexation model
6.) triple layer surface
     complexation model

The "activity" $K_d$ approach is the ratio of the amount of

metal adsorbed to the amount remaining in solution (ac-

tivity of the free ion). The $K_d$ equation can then be

written as follows:

$$K_d = \frac{SCu}{\{Cu\}} \qquad\qquad (4)$$

where:

$K_d$ = distribution coefficient
$SCu$ = particulate concentration (molal units)
$\{Cu\}$ = activity concentration of the free
     metal (molal units)

The "activity" Langmuir equation has an advantage over

the $K_d$ approach, because a mass balance on surface sites

is considered. The "activity" Langmuir equation is writ-

ten as follows:

$$SCu = \frac{K_L S_T \{Cu\}}{1 + K_L \{Cu\}} \qquad\qquad (5)$$

where:

$S_T$ = maximum quantity that can be adsorbed
$K_L$ = Langmuir adsorption constant

The third approach, the "activity" Freundlich, is used
when laboratory data obtained does not conform to the
"activity" Langmuir. The "activity" Freundlich equation
is written as follows:

$$SCu = K_f \{Cu\}^{1/n} \tag{6}$$

where:

$K_f$ = Freundlich adsorption constant
$n$ = a constant

The above three activity approaches are preferred over
their concentration counterparts, due to their ability to
deal with a wider range of natural waters. However, the
activity approach is not without limitations. The ac-
tivity approach does not charge balance surface sites and
adsorbed species. Secondly, electrostatic interactions
between adsorbing ion and charged surfaces are not con-
sidered. Finally, the reaction of solid with aqueous
constituents other then adsorbate ion is not considered.
In order to reduce the above limitations, surface com-
plexation models have been developed which may be more
applicable, but also more complex (Felmy et al., 1983).

The constant capacitance model and triple layer models, both based on theoretical approaches, consider charge potential differences and changing properties of the surface with changing pH and ionic strength. Both of these methods require a great deal of detailed laboratory investigation to determine the critical parameters and are primarily research tools.

The ion exchange approach is only useful when the selectivity coefficients for the exchange reactions are known. These coefficients are generally only available for bulk electrolyte ions such as sodium, potassium and calcium. The ion exchange model is inadequate for predicting metal adsorption, because metals usually form covalent bonds with surface sites (Felmy et al., 1983).

Finally, the equilibrium composition of an aquatic environment is determined by minimization of Gibbs free energy of the system within the mass balance constraints. This chemical equilibrium will determine metal speciation in addition to precipitation/dissolution and sorption, and is used in EXAMS to determine the metal fate and migration.

## 2.3 MEXAMS General Description

The two previous sections described the two individual models that have been linked to form the MEXAMS model (Figure 2). The MEXAMS program can be used
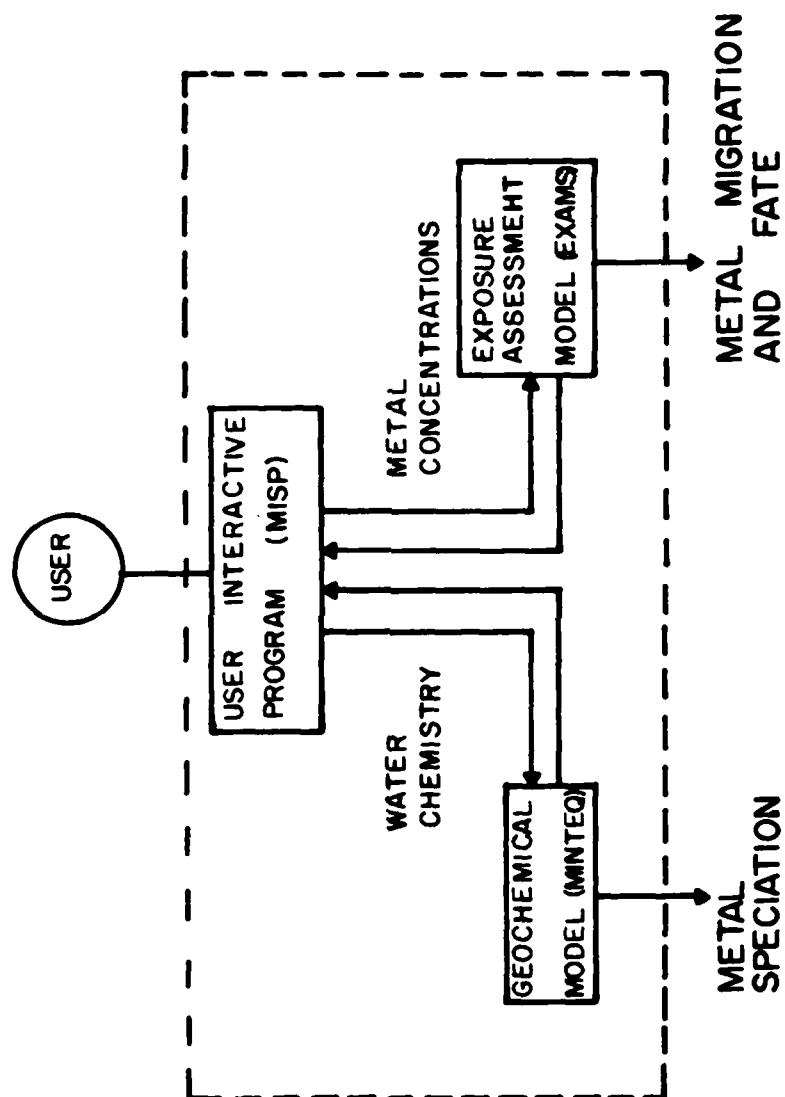
Figure 2.

in both batch and interactive mode with three different modes of operation available. The first mode is the MINTEQ only, which allows the operator to determine how changes in water chemistry will affect metal speciation and solid phase interactions without regard to transport processes. Secondly, the EXAMS only mode, which deals with the ionization, sorption, transport and transformation of a given pollutant. Finally, the third mode, which links EXAMS and MINTEQ together, allows the user to determine the effect of transport processes and chemical interactions on priority pollutant concentration. This section will describe the operation and use of the coupled mode.

The first step is to create an EXAMS input file that describes the characteristics of the aquatic environment being assessed. The user then enters the MEXAMS Interactive Software Package (MISP). MISP will call for a MINTEQ file for each compartment that contains different water quality data. The programmer will also input run-specific information that controls the number of times MINTEQ updates metal concentrations. MEXAMS is now set to simulate metal behavior, migration and fate.

Initial calculations by EXAMS are made assuming no adsorption or precipitation, and the initial distribution of dissolved metals in each compartment is obtained. These concentrations, along with suspended sediment and

biota concentrations, are sent on to MISP. MISP then passes the dissolved metal concentration in the first compartment on to MINTEQ, which simultaneously reads the water quality data for that compartment. MINTEQ then improves the estimate of the concentration of metal in solution, adsorbed to sediments and biota and in a precipitated form. These results are returned to MISP and metal fractions are determined.

MISP then proceeds to the second compartment and, unless the water quality is different and the total metal varies by more than 5%, MINTEQ is not called. MISP utilizes the same fractions from the previous compartment. If total metal varies by more than 5%, MINTEQ is called, but an entire new calculation is only performed when the water quality data differs from one compartment to the next.

After metal fractions have been computed for all compartments, MISP sends the information to EXAMS and the metal transport and transformation are computed. EXAMS then predicts new exposure levels and iterates with MINTEQ again. Calculations of fate and persistence are not performed until all iterations are complete.

EXAMS then sums the flux rate of metal attributable to each transport and transformation process, in which the significance of each process is then obtained by dividing flux rate by the total of the external

loadings. Finally, the persistence is calculated by terminating the external loading and computing the dissipation over two system half lives. In order to reduce computer time the two half lives have been divided into twelve equal time increments. Since metal concentration will change with time, the updating of each compartment metal fraction is possible. The user specifies the number of times the metal fractions are to be updated. The metal fractions will change with each time increment, and thus, after each persistence calculation they should be updated. The EXAMS output provides exposure, fate and persistence estimations, the MINTEQ output provides chemical interaction information and the MISP output provides information on EXAMS-MINTEQ interactions.

The MEXAMS computer program is capable of solving a wide variety of pollution problems. A list of possible uses follows:

1., Rapid evaluation of synthetic organic pollutants
2., Rapid hazard evaluation for priority pollutant metals
3.) Assess impact of point source discharge from mine drainage
4., Provide support interpretations of metal bioassays
5.) Framework for what is or what is not known about the behavior of priority pollutant metals in aquatic systems
6.) Management tool

Now that the three individual programs have been presented, the specific input files used for the

Naugatuck River will be discussed. This discussion will
include a description of the compartmentalized system
used, and a line by line explanation of the computer
inputs. The explanation will state any limitations, the
variable names and their computer format code. Some of
the parameters were not used in this report due to the
fact that the pollutants are priority metals, as opposed
to synthetic organic chemical contaminants.

CHAPTER 3

MODEL INPUTS AND OUTPUTS

## 3.1 Input Description (MINTEQ)

This section will present information regarding
the operation of the MINTEQ program. The MINTEQ program
has a great deal of flexibility in the way the user
defines the chemistry of the ecosystem being modeled. The
program is capable of dealing with six different specie
types, as described in the MINTEQ manual. The Type I
specie is the component. The component is defined as the
chemical specie chosen to represent each chemical con-
stituent. Each component corresponds to a MINTEQ iden-
tification (ID) number. Table 1 provides a complete list
of the components in MINTEQ. Type II complexes are
defined as aqueous species which are combinations of two
or more components. These complexes are not input by the
user, but instead are output by the computer as a result
of the Type I species input. Type III species are defined
as a species with a fixed activity.

Some examples of Type III species are components
at fixed activity such as pH or pE, solid phases present
in infinite supply, gases present at a fixed partial

## TABLE 1. COMPONENTS IN MINTEQ

| Component | I.D. Number | Component | I.D. Number |
|---|---|---|---|
| E | 001 | $NH_4^+$ | 490 |
| $H_2O$ | 002 | $NO_2^-$ | 491 |
| $Ag^+$ | 020 | $NO_3^-$ | 492 |
| $Al^{3+}$ | 030 | $Na^+$ | 500 |
| $H_3AsO_3$ | 060 | $Ni^{2+}$ | 540 |
| $H_3AsO_4$ | 061 | $PO_4^{3-}$ | 580 |
| $H_3BO_3$ | 090 | $Pb^{2+}$ | 600 |
| $Ba^{2+}$ | 100 | $Rb^+$ | 680 |
| $Br^-$ | 130 | $HS^-$ | 730 |
| $CO_3^{2-}$ | 140 | $S$ | 731 |
| Fulvate | 141 | $SO_4^{2-}$ | 732 |
| Humate | 142 | $H_4SiO_4$ | 770 |
| $Ca^{2+}$ | 150 | $Sr^{2+}$ | 800 |
| $Cd^{2+}$ | 160 | $U^{3+}$ | 890 |
| $Cl^-$ | 180 | $U^{4+}$ | 891 |
| $Cs^+$ | 220 | $UO_2^+$ | 892 |
| $Cu^{1+}$ | 230 | $UO_2^{2+}$ | 893 |
| $Cu^{2+}$ | 231 | | |
| $Fe^{2+}$ | 280 | | |
| $Fe^{3+}$ | 281 | | |
| $H^+$ | 330 | $Zn^{2+}$ | 950 |
| $I^-$ | 380 | SOH1 | 990 |
| $K^+$ | 410 | SOH2 | 991 |
| $Li^+$ | 440 | XPSIO | 992 |
| $Mg^{2+}$ | 460 | XPSIB | 993 |
| $Mn^{2+}$ | 470 | XPSID | 994 |
| $Mn^{3+}$ | 471 | SOHB | 995 |

(from Felmy et. al., 1983)

pressure, and redox reactions between two components. Type IV species are precipitated solids subject to complete dissolution. The Type III and Type IV solids are similar, except that Type IV solids have a finite mass. Type V species are dissolved solids subject to precipitation. These solid phases will only precipitate when the saturation index is exceeded. Finally, Type VI species are species not considered during equilibrium calculations. Instead, these species are considered after the equilibrium calculations are complete.

An example input file for the Naugatuck River is presented in Table 2, with the numbers on the left corresponding to line numbers, for explanation purposes. The first two lines are descriptive information for the sample site. The third line describes the water temperature (C), analytical units, and fixed ionic strength designation. If ionic strength is not to be fixed, 0.00 is input. Line four contains nine run specific user options, inorganic carbon input, debug print option, charge balance option, considered solids and print option, number of iterations, pH variation option, fixed ionic strength, numerical method selection and output option. The fifth line contains adsorption paramaters. Line six through 24 are the component input lines, and the three fields correspond to the specie ID number, total analytical mass and a guess for the log of the

TABLE 2

MINTEQ INPUT

```
 1.  NAUGATUCK RIVER CONDITIONS (16-17 AUGUST 1983)
     COMPARTMENT 1 ZN-CU-PB ADSORPTION
 2.  KD MODEL: MATRIX OBTAINED FROM BEST AVAILABLE
     DATA PH=7.14
 3.  25.00 MG/L    0.00
 4.  0 0 1 0 0 0 0 0
 5.  1   0.00    0.00    0.00    0.00
 6.       150 2.000E+01  -3.80
 7.       460 3.500E+00  -3.90
 8.       500 1.890E+01  -2.50
 9.       140 3.422E+01  -5.50
10.       732 2.500E+01  -2.90
11.       180 3.800E+01  -2.80
12.       090 8.361E-02  -5.10
13.       410 3.090E+00  -4.25
14.       580 4.906E-01  -11.0
15.       770 8.320E+00  -6.50
16.       231 5.450E-02  -9.00
17.       950 1.750E-02  -8.00
18.       492 7.083E+00  -8.00
19.       470 3.550E-02  -7.00
20.       281 2.140E-01  -7.00
21.       600 6.000E-03  -8.00
22.       330 0.000E-00  -7.14
23.       991 0.000E-00   0.00
24.       990 0.000E+00   0.00
25.
26.    3   3
27.       330       7.14
28.       990
29.       991
30.
31.    2   3
32.  9909500 SOH-ZN                        -.24
33.       2    1.00 950    1.00 990
34.
35.  9916000 SOH-PB                        1.33
36.       2    1.00 600    1.00 991
37.
38.  9912310 SOH-CU                        0.20
39.       2    1.00 231    1.00 991
40.
41.
```

component activity. This section is the water quality
data for each compartment of the ecosystem. The water
quality data for the Naugatuck River was obtained from
three sources (A.J. Medine et al., 1982, Curtis 1982, and
USGS Water Resources Data-Connecticut, 1982). The water
quality data used is presented in Table 3. The next line
is a blank line separating specie Type I from specie Type
III. Line 26 corresponds to the specie type and the
number of species of that type. The next three lines are
for fixed pH and two surface sites for adsorption. After
another blank line, the adsorption information is input.
This input section consists of nine lines. The first line
contains the type of modification and number of these
modifications. Then each adsorption input has three
corresponding lines of input. The first line is the
adsorption description and the log $K_d$ value for the
reaction.

The adsorption routine chosen in this case was
the "activity" $K_d$ approach. The log $K_d$ values were ob-
tained by running the MINTEQ program without adsorption.
By using the activity results and the field-observed
particulate concentration for each metal in Equation 4,
the "activity" $K_d$ was obtained (log $K_d$ was then utilized
as an input to the program). Table 4 presents the data
obtained for each compartment, and the respective $K_d$
values. The second line corresponds to the components and

Table 3

Water Quality Data

| Component | Concentration (mg/l) | Data Source |
|---|---|---|
| 150 - Ca | 1.50 E+01 | U.S.G.S. (1983) |
| 460 - Mg | 3.50 E+00 | U.S.G.S. (1983) |
| 500 - Na | 1.89 E+01 | Medine & Conway (1982) |
| 410 - K | 3.09 E+00 | Medine & Conway (1982) |
| 470 - Mn | * | Conn. - DEP (1982)** |
| 281 - Fe | * | Conn. - DEP (1982)** |
| 770 - SiO2 | 8.32 E+00 | U.S.G.S. (1983) |
| 950 - Zn | * | Conn. - DEP (1982)** |
| 090 - B | 8.36 E-02 | Medine & Conway (1982) |
| 231 - Cu | * | Conn. - DEP (1982)** |
| 732 - SiO4 | 2.50 E+01 | U.S.G.S. (1982) |
| 180 - Cl | 3.80 E+01 | U.S.G.S. (1982) |
| 140 - CO3 | 3.42 E+01 | Medine & Conway (1982) |
| 492 - NO3 | 7.08 E+00 | U.S.G.S. (1982) |
| 580   PO4 | 4.91 E-01 | U.S.G.S. (1982) |
| 600 - Pb | * | Conn. - DEP** |
| 330 - H | * | Conn. - DEP** |

*These inputs are compartment dependent
**Connecticut State Department of Environmental
  Protection

TABLE 4

Compartment Kd Data

| Compart- ment #-Type | Element | Free Ion Activity (M) | Particulate Conc. (M) | Log Kd |
|---|---|---|---|---|
| 1-E | Cu | 9.741 E-08 | 1.50 E-07 | .20 |
|  | Pb | 9.940 E-10 | 2.17 E-08 | 1.23 |
|  | Zn | 1.321 E-07 | 7.65 E-08 | -.24 |
| 2-B | Cu | 8.467 E-07 | 4.41 E-03 | 3.73 |
|  | Pb | 9.300 E-07 | 2.79 E-03 | 3.48 |
|  | Zn | 5.451 E-05 | 3.89 E-03 | 1.85 |
| 3-E | Cu | 1.634 E-07 | 1.34 E-07 | -.09 |
|  | Pb | 2.551 E-09 | 2.17 E-08 | .93 |
|  | Zn | 1.830 E-07 | 9.94 E-08 | -.26 |
| 4-B | Cu | 1.796 E-06 | 1.59 E-03 | 2.95 |
|  | Pb | 1.834 E-06 | 3.00 E-04 | 2.21 |
|  | Zn | 4.637 E-05 | 3.49 E-03 | 1.88 |
| 5-E | Cu | 4.422 E-08 | 3.93 E-08 | -.05 |
|  | Pb | 2.234 E-09 | 2.17 E-08 | .99 |
|  | Zn | 9.065 E-08 | 5.35 E-08 | -.23 |
| 6-B | Cu | 3.225 E-06 | 1.51 E-03 | 2.67 |
|  | Pb | 2.543 E-06 | 3.07 E-04 | 2.08 |
|  | Zn | 2.177 E-05 | 3.66 E-03 | 2.23 |

E - Eplimnion
B - Benthic

the stoichiometry of the reaction. Finally, the next two lines are blank to signify the end of the input file.

This section described the input file for the Naugatuck River. Also included in the appendices is a copy of the MINTEQ input description (Felmy et al., 1983). This description includes computer format, possible options and a more in-depth description of the MINTEQ input file itself. Following the input of the MINTEQ data file, the next step is the creation of an EXAMS input file.

## 3.2 Input Description (EXAMS)

The EXAMS input file is generated based on a compartmentalization of the riverine ecosystem. EXAMS, as stated previously, is responsible for the metal fate and migration calculations. Figure 3 displays the initial compartmentalization scheme used for the Naugatuck River system. Once the compartmentalization is selected, the EXAMS input file is generated. The file consists of 67 lines of input, which will be explained next (Table 5).

The first two lines are descriptive lines for the ecosystem, the chemical name and ecosystem name, both a maximum of three characters. The third line corresponds to the number of chemical loadings. In this case, there are five loadings and the next five lines describe the loading as one of five types (units of input for each

COMPARTMENTALIZATION

KEY:

① – COMPARTMENT #'s

→ – ADVECTIVE PATHWAYS

⇢ – DISPERSIVE PATHWAYS

Ⓐ – POINT SOURSE LOADINGS

⥣ – GROUNDWATER SEEPAGE

Figure 3.

## Table 5

### EXAMS Input

```
NAG
  5
  1 1.264E-02        0.        0.        0.        0.
  2      0.          0.        0.        0. 6.505E-04
  3 4.404E-03        0.        0.        0.        0.
  5 3.361E-02        0.        0.        0.        0.
  6      0.          0.        0.        0. 3.538E-04
HVM
Heavy Metal
0 0 0 0 0
NAG
NAUGATUCK RIVER CALIBRATION TEST RUN
    6
L
B
L
B
L
E
 41.80
 0.0000    0.0000     0.0000     0.0000     0.0000     0.0000
 9.316E+03 4.925E+02 3.353E+03 1.149E+02 7.903E+04 2.402E+03
 5.366E+04 5.386E+04 1.257E+04 1.257E+04 2.627E+05 2.627E+05
 0.17069   0.00914   0.17963   0.00914   0.3048    0.00914
 9.658E+02 0.000     4.694E+01 0.000     7.708E+02 0.000
 2.9668    0.000     0.489     0.000     5.528     0.000
 0.000     0.000     0.000     0.000     0.000     0.000
 0.000     0.000     0.000     0.000     0.000     0.000
 1.625E+02 1.625E+02 0.000     0.000     3.538E+02 3.538E-02
 00.00
 100.0
 0.000     0.000     0.000     0.000     0.000     0.000     0.000    0.000
 0.000     0.000     0.000     0.000     0.000     0.000     0.000    0.000
 0.000     0.000     0.000     0.000     0.000     0.000     0.000    0.000
 0.000     0.000     0.000     0.000     0.000     0.000     0.000    0.000
 0.000     0.000     0.000     0.000     0.000     0.000     0.000
       00.00     00.00     00.00     00.00     00.00     00.00
       00.00     00.00     00.00     00.00     00.00     00.00
 3.000     1.530     3.000     1.530     7.500     1.530
 0.000     115.2     0.000     115.2     0.000     115.2
    6
    1     3     5     2     4     4     6     2
    3     5     0     1     3     6     5     4
 1.000     1.000     1.000     0.900     0.900     0.100     1.000    0.100
    3
    1     3     5
    2     4     6
 5.386E+04 1.257E+04 2.627E+04
 8.992E-02 9.449E-02 1.570E-01
 5.000E-07 5.000E-07 5.000E-07
 0.3800E-01 0.3800E-01 0.3800E-01 0.3800E-01 0.3800E-01 0.3800E-01
 25.00     25.00     25.00     25.00     25.00     25.00
 25.00     25.00     25.00     25.00     25.00     25.00
 23.50     23.50     23.50     23.50     23.50     23.50
 7.143     7.143     7.007     7.007     7.078     7.078
 6.857     6.857     6.993     6.993     6.922     6.922
 0.1000E-08          0.00.1000E-080.5000E-09          0.00.1000E-08
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
 23.50     23.50     23.50     23.50     23.50     23.50
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
 00.00     00.00     00.00     00.00     00.00     00.00
```

chemical loading are Kg/hr). The five types of loadings
are point source, non-point source, rainfall, aerial
drift and ground water seepage. The loadings are input
from left to right for each compartment in the order
previously stated. The next two lines are a description
of the chemical, followed by a line of flags denoting
which species of the organic toxicant can occur. A zero
is used for no occurrence and a one for occurrence, and
in this case, zeros are input because the pollutant being
investigated is a heavy metal. The next two lines are an
ecosystem description.

The ecosystem was divided into unequal compart-
ment lengths representing well-defined segments based on
actual point loadings. Compartments one and two are 1.3
miles long, compartments three and four are .3 miles long
and compartments five and six are 6.7 miles long. Figure
4 displays the four different sample sites (East Albert
St., Gulf Stream, Bogue Road, Bridge Abutment) within the
stream segment selected for compartmentalization and
modeling.

The next seven lines are the number of compart-
ments, and the compartment code for each compartment. The
compartments are classified as epilimnion (E), hypolim-
nion (H), littoral (L) or benthic (B). The compartment
classification is then followed by the latitude input in
degrees, and the wind velocity at 10 cm above the water

NAUGATUCK RIVER



APPROX. SCALE: 1" ≈ 10 KILOMETERS
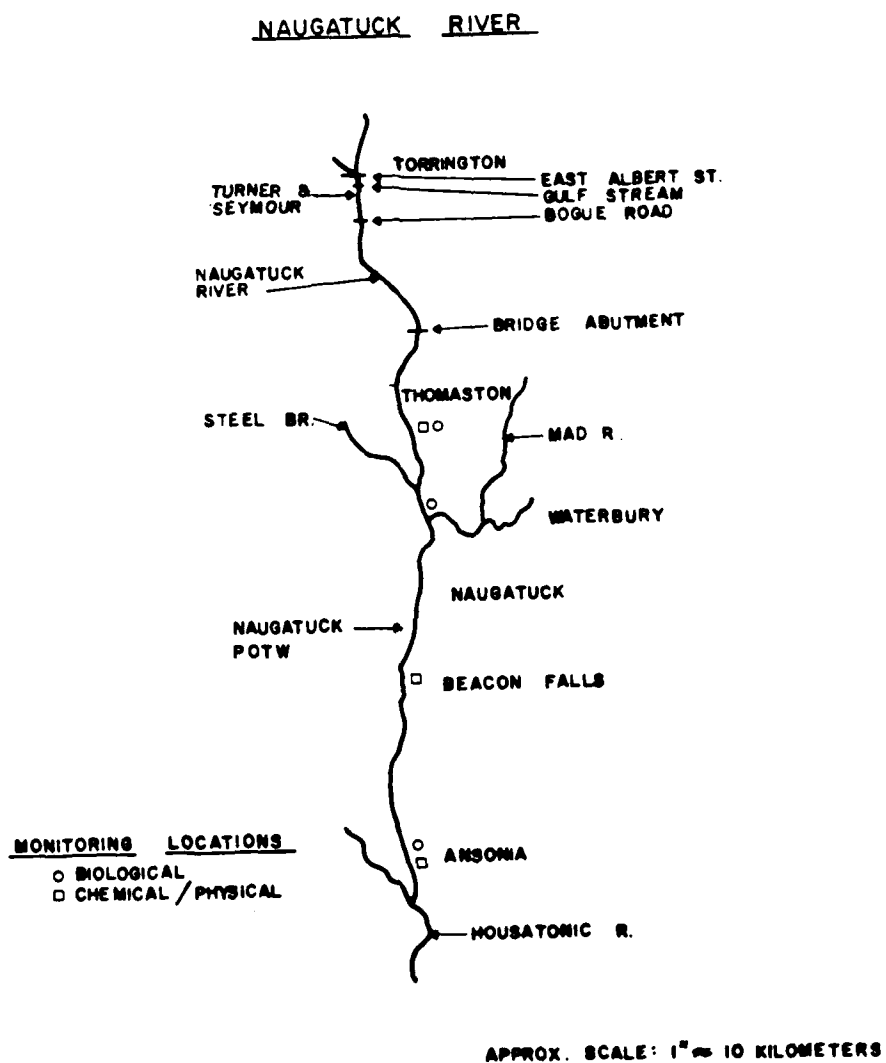
Figure 4.

surface ₁m/sec₁ for each compartment. Line 24 is the
environmental volume (cubic meters) for each compartment
followed by entries of area (square meters₁ and average
depth (m) for each compartment.

The next section, lines 27 through 31, represent
flows entering the ecosystem compartments. These flows
are of the following type: stream flow ₁cubic meters/hr₁,
stream-born sediment load ₁Kg/hr), non-point source water
flow ₁cubic meters/hr₁, non-point source sediment loads
(Kg/hr), and ground water seepage flow (cubic meters/hr).
The next input is average rainfall (mm/mo) in the
geographic area, then the average cloudiness in tenths of
full sky cover is input. From this point on in the data
set, many parameters are input as zero because they deal
with transformation of organic toxicants and not priority
pollutant heavy metals.

The next six lines are inputs for average
spectral irradiance immediately below the water surface.
These inputs are not required for transformation of heavy
metals. Line 40 corresponds to the evaporative water
losses (mm/mo) from each compartment. The next line is
where suspended sediment concentrations (mg/l) are input
if dealing with water column compartments and bulk den-
sity (g/cc) for benthic compartments. These inputs are
followed by percent water in bottom sediments of benthic
compartments. Water column compartments have inputs of

zero for this variable.

The transport mechanisms of advection and dispersion are input in lines 43 - 52. Advection is input first, with the first line corresponding to the number of advective pathways. The next three lines are the source compartment, the receiving compartment and the proportion of the advective flow. The dispersive pathways are then input. The first line equates to the number of dispersive pathways. The source compartments are then entered followed by the receiving compartment and the description of the exchange pathway. The cross-sectional area (square meters), characteristic length (m) and eddy dispersion coefficients (square meters/hr) are the parameters required to describe the dispersive pathway. The characteristic length is defined as the distance from compartment center to compartment center.

The next three lines correspond to the organic carbon content of compartment sediment, cation and anion exchange capacity of the sediments. Line 56 is the average temperature for each compartment. The pH and pOH of each compartment are the next two inputs. Finally, the remaining lines are not required for the modeling of the Naugatuck riverine ecosystem for the migration and fate of priority pollutant metals.

Included in the appendices is a copy of the EXAMS input file description (Burns et al., 1981). The descrip-

tion provides a detailed description of the computer format, and the parameters which were not used, but can be used for organic toxicants.

For each compartment there is a corresponding MINTEQ input file, and it should be re-emphasized that each compartment is assumed to be completely mixed after the priority pollutant enters the compartment. After input files have been created for each compartment (MINTEQ), and the transformation and transport model (EXAMS) input file is complete, the MISP interactive input file is created.

This file encompasses twenty-five lines in this example. These lines allow the interaction of MINTEQ with EXAMS and produce the MEXAMS system model. The first line corresponds to the selection of the computer mode (MINTEQ only, or coupled version). The metal selection is made next from the list of metals (As, Cd, Cu, Pb, Ni, Ag and Zn) and corresponding identification numbers in the MINTEQ components list. The next line corresponds to how many MINTEQ files are needed. The number of required files is dependent on the water quality data for the aquatic system. If the water quality data does not change significantly for each compartment, then one file is sufficient. Water quality fluctuations could be a result of wastewater treatment plant discharges, industrial discharges, overland runoff, etc.

The next group of lines corresponds to the number of compartments that match up with each MINTEQ file, followed by the compartment number that corresponds to each MINTEQ file. The next input is the number of times the programmer wants the steady state metal concentration updated. EXAMS initially assumes all metal is in the dissolved form and by providing MINTEQ with these results, the actual dissolved, sediment sorbed, biosorbed and precipitated metal concentrations are obtained. EXAMS uses these updated calculations in the next simulation for fate and transport of the pollutant. Line seventeen relates to how often MINTEQ is used for persistence calculations. After steady state has been achieved, the pollutant loading is ceased and persistence calculations begin. These calculations are based on two system half-lives, which are divided into twelve equal time increments. This input will continue metal fraction updating throughout the persistence calculations. The next three inputs correspond to the output option, the MINTEQ file names for each compartment, and the EXAMS input file name. There are three output options available: the full MINTEQ output, aqueous species distribution and all mass totals, and all mass totals. This concludes the MISP interactive input file. Table 6 is a sample of the MISP file.

3.3 Output (MINTEQ)

Table 6

MISP Input

```
3
231
6
1
1
1
2
1
3
1
4
1
5
1
6
3
4
3
NAUG1.DAT
NAUG2.DAT
NAUG3.DAT
NAUG4.DAT
NAUG5.DAT
NAUG6.DAT
EXAMS21.DAT
```

The MINTEQ output data received when the un-
coupled mode is operated can be divided into seven sec-
tions. The first section is a duplication of the first
five lines of the input file. Section two corresponds to
the initial charge balance of the solution being modeled,
prior to aqueous speciation. A large percent difference
can be indicative that one or more major cations or
anions may have been neglected when preparing the water
quality input file. However, the water analysis may be
entirely correct with the final speciation indicating an
acceptable charge balance. Therefore, initial charge
imbalance should be evaluated on a case by case basis
(section 2 is presented in Table 7).

The third section provides an iterative output
displaying the convergence of the first component in the
input file to its actual speciated activity (Table 7).
Also included in this section is the calculated molality,
activity, Log activity, activity coefficient, and new Log
K for all input components. The new Log K is the effec-
tive equilibrium constant after temperature and ionic
strength corrections. This section can be used to enable
the user to make a better guess for the activity in the
input file.

The fourth section provides the output data for
the six different specie types. The output for Type I
components and Type II complexes are similar with the

Table 7

MINTEQ Output

CHARGE BALANCE: UNSPECIATED
SUM OF CATIONS= 2.203E-03 SUM OF ANIONS = 2.863E-03
PERCENT DIFFERENCE = -13.04   (CATIONS - ANIONS)/(ANIONS + CATIONS)

ITERATIONS DURING SOLVE

| ITER | NAME | TOTAL MOL | DIFF FXN | LOG ACTVTY |
|------|------|-----------|----------|------------|
| 1 | CA | 4.991E-04 | -2.910E-04 | -3.80000 |
| 2 | CA | 4.991E-04 | -6.766E-05 | -3.38469 |
| 3 | CA | 4.991E-04 | 1.439E-04 | -3.32420 |
| 4 | CA | 4.991E-04 | 2.858E-04 | -3.43010 |
| 5 | CA | 4.991E-04 | -1.933E-04 | -3.62025 |
| 6 | CA | 4.991E-04 | 3.429E-06 | -3.41555 |

OUTPUT DATA:  ITERATIONS = 6

| ID | NAME | ANAL MOL | CALC MOL | ACTIVITY | LOG ACTVTY | GAMMA | NEW LOGK | DIFF FXN |
|-----|------|----------|----------|----------|------------|--------|----------|----------|
| 150 | CA | 4.991E-04 | 4.815E-04 | 3.817E-04 | -3.41830 | .792686 | .1009 | -3.620E-07 |
| 460 | MG | 1.440E-04 | 1.393E-04 | 1.107E-04 | -3.95593 | .794378 | .1000 | -1.034E-07 |
| 500 | NA | 8.222E-04 | 8.211E-04 | 7.734E-04 | -3.11159 | .941939 | .0260 | -1.644E-07 |
| 140 | CO3 | 5.703E-04 | 3.792E-07 | 2.996E-07 | -6.52348 | .789951 | .1024 | -9.605E-08 |

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following headings: calculated molality, activity, Log activity, activity coefficient (GAMMA), new Log K, and the enthalpy of the reaction (DH). Type III fixed solids are of four basic categories, redox reactions, components at fixed activity, solid phases and gases at a fixed partial pressure. The output for these type species consists of calculated molality, Log molality, new Log K and the DH. In our case the Type III species fall into the category of fixed activities, thus any intuitive information from this section cannot be obtained. However, if solid phases were being dealt with, a positive calculated molality would equal the mass of solid precipitated. On the other hand, a negative calculated molality would equal the dissolved mass or mass added to the solution. No Type IV or Type V species were permitted from the list of solids which were supersaturated as indicated by MINTEQ. Chemical precipitation has not been observed in the Naugatuck River although it cannot be precluded. Type V calculated molality would correspond to saturation index values. Type VI has two different interpretations for the calculated molality. If solid phase, it corresponds to saturation index. If aqueous species, it corresponds to activity of specie. A sample of section four output is displayed in Table 8.

Section five presents the percentage distribution of Type I components and Table 9 is an example. The sixth

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## Table 8

### MINTEQ Output

```
SPECIES   TYPE  I - COMPONENTS
ID        NAME      CALC MOL    ACTIVITY    LOG ACTVTY   GAMMA      NEW LOGK    DH
  150   CA          4.815E-04   3.817E-04   -3.41830    .792686      .101       0
  460   MG          1.393E-04   1.107E-04   -3.95593    .794378      .100       0
  500   NA          8.211E-04   7.734E-04   -3.11159    .941939      .026       0
  140   CO3         3.792E-07   2.996E-07   -6.52348    .789951      .102       0
  732   SO4         2.408E-04   1.891E-04   -3.72333    .785348      .105       0
  180   CL          1.072E-03   1.008E-03   -2.99650    .940572      .027       0
   90   H3BO3       1.341E-06   1.342E-06   -5.87224   1.000697     -.000       0
  410   K           7.892E-05   7.423E-05   -4.12945    .940572      .027       0
  580   PO4         1.940E-11   1.137E-11  -10.94412    .586236      .232       0
  770   H4SIO4      8.643E-05   8.649E-05   -4.06305   1.000697     -.000       0
  231   CU+2        1.223E-07   9.686E-08   -7.01385    .791776      .101       0
  950   ZN          1.671E-07   1.323E-07   -6.87842    .791776      .101       0
  492   NO3         1.142E-04   1.074E-04   -3.96888    .940473      .027       0
  470   MN+2        6.220E-07   4.925E-07   -6.30758    .791776      .101       0
  281   FE+3        1.245E-14   7.545E-15  -14.12233    .606033      .218       0
  600   PB          1.286E-09   1.010E-09   -8.99549    .785813      .105       0

SPECIES   TYPE  II - COMPLEXES
ID        NAME      CALC MOL    ACTIVITY    LOG ACTVTY   GAMMA      NEW LOGK    DH
1503300   CAOH +     1.409E-09   1.329E-09   -8.87633    .943302   -12.573    14.535
1501400   CAHCO3 +   1.944E-06   1.834E-06   -5.73669    .943302    11.370     1.790
1501401   CACO3 AO   1.624E-07   1.625E-07   -6.78917   1.000697     3.152     4.030
1507320   CASO4 AQ   1.469E-05   1.470E-05   -4.83263   1.000697     2.309     1.470
1505800   CAHPO4 AO  3.822E-07   3.825E-07   -6.41742   1.000697    15.085     -.230
1505801   CAPO4 -    1.325E-08   1.249E-08   -7.90342    .942758     6.485     3.100
1505802   CAH2PO4 +  2.204E-08   2.078E-08   -7.68242    .942758    20.986    -1.120
5001400   NACO3 -    4.555E-09   4.295E-09   -8.36707    .942758     1.294     8.911
5001401   NAHCO3 AO  2.017E-07   2.018E-07   -6.69507   1.000697    10.080       0

6001800   PBCL +     4.307E-11   4.055E-11  -10.39199    .941520     1.626     4.380
6001801   PBCL2 AQ   6.475E-14   6.479E-14  -13.18849   1.000697     1.800     1.080
6001802   PBCL3 -    5.498E-17   5.176E-17  -16.28599    .941520     1.725     2.170
6001803   PBCL4 -2   3.186E-20   2.503E-20  -19.60149    .785813     1.485     3.530
6001400   PB(CO3)2-2 5.006E-12   3.959E-12  -11.40245    .785813    10.745       0
6003300   PBOH +     2.388E-10   2.710E-10   -9.56552    .941520    -7.684       0
6003301   PB(OH)2 AQ 1.459E-12   1.460E-12  -11.83554   1.000697   -17.120       0
6003302   PB(OH)3 -  2.458E-16   2.314E-16  -15.63557    .941520   -28.034       0
6003303   PB2OH +3   1.058E-17   6.152E-18  -17.21101    .581390    -6.124       0
6004920   PBNO3 +    1.705E-12   1.606E-12  -11.79437    .941520     1.196       0
6007320   P3SO4 AQ   1.074E-10   1.074E-10   -9.96882   1.000697     2.750       0
6003304   PB3(OH)4+2 6.282E-23   4.937E-23  -22.30658    .785813   -23.775    26.500
6001401   PBCO3 AQ   5.257E-09   5.261E-09   -8.27897   1.000697     7.240       0
6003305   PB(OH)4 -2 9.334E-21   7.335E-21  -20.13460    .785813   -39.594       0
6007321   PB(SO4)2-2 1.357E-13   1.066E-13  -12.97214    .785813     3.575       0

SPECIES   TYPE  III - FIXED SOLIDS
ID        NAME      CALC MOL     LOG MOL    NEW LOGK     DH
    2   H2O        -9.247E-06   -5.034      .000         0
  991   SOH2       -1.751E-07   -6.757      0            0
  990   SOH1       -7.613E-08   -7.118      0            0
  330   H          -6.425E-04   -3.192     7.140         0

SPECIES   TYPE  VI - SPECIES NOT CONSIDERED
ID        NAME      CALC MOL     LOG MOL    NEW LOGK     DH
3301403   CO2(GAS)   2.273E-03   -2.643     18.160      -.530
```

section presents the amount of each Type I component in solution (aqueous mass), sorbed (sorbed mass) and precipitated (precipitated mass). The final charge balance is also presented, and if the final percent difference after aqueous speciation is less than five percent, the run is acceptable. A sample of section six output is presented in Table 9. The heavy metal under investigation in this case study is copper, and from Table 9 it can be seen that 14.3 percent of the copper is in the free ion form, 16.9% bound to surface sites with the remainder as inorganic complexes.

The final section provides the saturation indices for all minerals and solids in the data base. This section is used to determine if the saturation index of a particular mineral or solid has been exceeded. A positive Log SI means the solid is oversaturated. This also tells you that this solid could precipitate, and thus, if your environment favors this solid, the solid could be input as a Type IV solid and allowed to precipitate. Finally, a line will be printed "NORMAL TERMINATION OF MINTEQ" and the output is complete. The final section is presented in Table 10. An example of the entire MINTEQ output is presented in the appendices.

## 3.4 Output (EXAMS)

The EXAMS output obtained when the coupled mode

## Table 9

### MINTEQ Output

**PERCENTAGE DISTRIBUTION OF COMPONENTS**

CA

| | | |
|---|---|---|
| 96.5 | PERCENT BOUND IN SPECIES  150 | CA |
| 2.9 | PERCENT BOUND IN SPECIES 1507320 | CASO4 AQ |

CU+2

| | | |
|---|---|---|
| 14.3 | PERCENT BOUND IN SPECIES  231 | CU+2 |
| 17.9 | PERCENT BOUND IN SPECIES 9912310 | SOH-CU |
| 18.2 | PERCENT BOUND IN SPECIES 2311400 | CUCO3 AQ |
| 1.7 | PERCENT BOUND IN SPECIES 2313300 | CUOH + |
| 44.9 | PERCENT BOUND IN SPECIES 2313301 | CU(OH)2 AQ |
| 2.6 | PERCENT BOUND IN SPECIES 2311402 | CUHCO3 + |

ZN

| | | |
|---|---|---|
| 62.4 | PERCENT BOUND IN SPECIES  950 | ZN |
| 2.2 | PERCENT BOUND IN SPECIES 9507320 | ZNSO4 AQ |
| 2.9 | PERCENT BOUND IN SPECIES 9501400 | ZNHCO3 + |
| 3.0 | PERCENT BOUND IN SPECIES 9501401 | ZNCO3 AQ |
| 28.4 | PERCENT BOUND IN SPECIES 9909500 | SOH-ZN |

| IDX | NAME | AQUEOUS MASS | SORBED MASS | PRECIPITATED MASS |
|---|---|---|---|---|
| 150 | CA | 4.987E-04 | 0 | 0 |
| 460 | MG | 1.430E-04 | 0 | 0 |
| 500 | NA | 9.221E-04 | 0 | 0 |
| 140 | CO3 | 5.702E-04 | 0 | 0 |
| 732 | SO4 | 2.601E-04 | 0 | 0 |
| 180 | CL | 1.072E-03 | 0 | 0 |
| 90 | H3BO3 | 1.352E-06 | 0 | 0 |
| 410 | K | 7.902E-05 | 0 | 0 |
| 580 | PO4 | 5.184E-06 | 0 | 0 |
| 770 | H4SIO4 | 8.658E-05 | 0 | 0 |
| 231 | CU+2 | 7.042E-07 | 1.535E-07 | 0 |
| 950 | ZN | 1.915E-07 | 7.613E-08 | 0 |
| 492 | NO3 | 1.142E-04 | 0 | 0 |
| 470 | MN+2 | 6.438E-07 | 0 | 0 |
| 281 | FE+3 | 3.832E-06 | 0 | 0 |
| 600 | PB | 7.360E-09 | 2.160E-08 | 0 |
| 2 | H2O | 9.247E-06 | 0 | 0 |
| 330 | H | 6.425E-04 | 0 | 0 |

CHAPGE BALANCE  SPECIATED

SUM OF CATIONS = 2.149E-03 SUM OF ANIONS  2.168E-03
PERCENT DIFFERENCE =   -.43  (CATIONS - ANIONS)/(ANIONS + CATIONS)
NONCARBONATE ALKALINITY =  0
IONIC STRENGTH =  3.026E-03

Table 10

MINTEQ Output

SATURATION INDICES FOR ALL MINERALS AND SOLIDS

| ID | NAME | LOG SI | LOG K | MIN LOGK | MAX LOGK | LOG IAP | DH |
|---|---|---|---|---|---|---|---|
| 6015000 | ANHYDRITE | -2.505 | 4.637 | 0 | 0 | -7.142 | 3.769 |
| 5015000 | ARAGONITE | -1.606 | 8.336 | 0 | 0 | -9.942 | 2.615 |
| 5046000 | ARTINITE | -9.755 | -9.600 | 0 | 0 | -.155 | 28.742 |
| 2046000 | BRUCITE | -6.463 | -16.792 | 0 | 0 | 10.324 | 25.840 |
| 5015001 | CALCITE | -1.467 | 8.475 | 8.560 | 0 | -9.942 | 2.585 |
| 2077000 | CHALCEDONY | -.540 | 3.523 | 0 | 0 | -4.063 | -4.615 |
| 8646000 | CHRYSOTILE | -9.042 | -32.188 | 0 | 0 | 22.846 | 52.485 |
| 8246000 | CLINOENSTITE | -5.077 | -11.336 | -10.972 | -11.632 | 6.261 | 20.015 |
| 2077001 | CRISTOBALITE | .476 | 3.587 | 0 | 0 | -4.063 | -5.500 |
| 8215000 | DIOPSIDE | -6.826 | -19.886 | 0 | 0 | 13.060 | 32.280 |
| 5015002 | DOLOMITE | -3.421 | 17.000 | 0 | 0 | -20.421 | 8.290 |
| 6046000 | EPSOMITE | -5.539 | 2.140 | 0 | 0 | -7.679 | -2.820 |
| 8646003 | SEPIOLITE(C) | -7.454 | -15.913 | 0 | 0 | 8.459 | 27.268 |
| 2028100 | FERRIHYDRITE | 2.407 | -4.891 | -1.557 | -4.996 | 7.298 | 0 |
| 4128100 | FE(OH)2.7CL.3 | 7.297 | 3.040 | 0 | 0 | 4.257 | 0 |
| 6028100 | FE2(SO4)3 | -42.995 | -3.580 | .650 | 0 | -39.415 | 59.120 |
| 8046000 | FORSTERITE | -11.713 | -28.298 | 0 | 0 | 16.585 | 48.510 |
| 2026102 | GOETHITE | 6.798 | .500 | 0 | 0 | 7.298 | 14.480 |
| 6015001 | GYPSUM | -2.294 | 4.848 | 0 | 0 | -7.142 | -.261 |
| 4150000 | HALITE | -7.690 | -1.582 | 0 | 0 | -6.108 | -.918 |
| 3028100 | HEMATITE | 18.603 | 4.008 | 0 | 0 | 14.595 | 30.845 |
| 5015003 | HUNTITE | -11.412 | 29.968 | 0 | 0 | -41.380 | 25.760 |
| 5046001 | HYDRMAGNESIT | -22.828 | 8.766 | 0 | 0 | -31.594 | 52.210 |
| 6050000 | JAROSITE NA | 1.115 | 11.200 | 0 | 0 | -10.085 | 36.180 |
| 8215002 | WOLLASTONITE | -6.197 | -12.996 | 0 | 0 | 6.799 | 19.498 |
| 8215003 | P-WOLLSTANIT | -7.047 | -13.846 | 0 | 0 | 6.799 | 21.068 |
| 8015001 | CA-OLIVINE | -19.989 | -37.649 | 0 | 0 | 17.660 | 54.695 |
| 8015002 | LARNITE | -21.481 | -39.141 | 0 | 0 | 17.660 | 57.238 |
| 6015007 | CA3SIO5 | -45.345 | -73.867 | 0 | 0 | 28.522 | 106.335 |
| 8015003 | MONTICELLITE | -13.149 | -20.272 | 0 | 0 | 17.123 | 49.421 |
| 8015005 | AKERMINITE | -23.551 | -47.472 | 0 | 0 | 23.921 | 76.445 |
| 8015004 | MERWINITE | -33.760 | -68.543 | 0 | 0 | 34.783 | 107.111 |
| 3028102 | LEPIDOCROCIT | 5.927 | -1.371 | 0 | 0 | 7.298 | 0 |

NORMAL TERMINATION OF MINTEQ

is selected is dependent upon the MISP file configuration. The parameter which controls the EXAMS output is the number of times EXAMS uses MINTEQ to update steady state metal concentrations. EXAMS utilizes MINTEQ three times to update steady-state metal concentrations in the Naugatuck River test case. The selection of this parameter is based on trial and error; the programmer examines the output obtained while varying the input and determines when system steady state is achieved. System steady state is defined as an equilibrium between the partioning achieved with EXAMS and MINTEQ.

The EXAMS output file received after each steady state calculation will be divided into three sections. The first section consists of 13 tables, which were obtained from the initial EXAMS calculation. The initial EXAMS calculation assumes the pollutant is in the aqueous form. Tables 2 - 8 (all shown in Table 11) are echoes of the EXAMS input data. Table 1 is not printed because the pollutant in question is a heavy metal and not an organic. If the pollutant had been an organic, Table 1 would have been an echo of the organic input data.

The next section includes Tables 9 - 14 (all shown in Table 12). These five tables are the transport profile, the kinetic profile, the canonical profile, toxicant loadings by system element, the distribution of the chemical at steady state (the water column and

Table 11

EXAMS Output

```
ECOSYSTEM: NAUGATUCK RIVER CALIBRATION TEST RUN
---------------------------------------------------------------
 TABLE 2.  INPUT DATA DESCRIBING ENVIRONMENT: GLOBAL PARAMETERS.
---------------------------------------------------------------
 KOUNT= 10    RAIN(MM/MO)=  .0    CLOUD(10THS)=  1.0E+02 LAT= 41.80
 IRRADIANCE (WLAM,P/SQ CM/SEC/N NM):
  .0       .0       .0       .0       .0
  .0       .0       .0       .0       .0
  .0       .0       .0       .0       .0
  .0       .0       .0       .0       .0
  .0       .0       .0       .0       .0
---------------------------------------------------------------
```

Table 11 (continued)

TABLE 3. INPUT DATA DESCRIBING ENVIRONMENT: BIOLOGICAL PARAMETERS.

| # TY | BIOMS (1) | PLRA (2) | BIOTM DEG C. | BACTO (3) | ACBAC (2) | CHL MG/L |
|------|-----------|----------|--------------|-----------|-----------|----------|
| 1L   | .0        | .0       | 23.50        | .0        | .0        | .0       |
| 2B   | .0        | .0       | 23.50        | .0        | .0        |          |
| 3L   | .0        | .0       | 23.50        | .0        | .0        | .0       |
| 4B   | .0        | .0       | 23.50        | .0        | .0        |          |
| 5L   | .0        | .0       | 23.50        | .0        | .0        | .0       |
| 6B   | .0        | .0       | 23.50        | .0        | .0        |          |
| 7L   | .0        | .0       | 23.50        | .0        | .0        | .0       |
| 8B   | .0        | .0       | 23.50        | .0        | .0        |          |
| 9L   | .0        | .0       | 23.50        | .0        | .0        | .0       |
| 10B  | .0        | .0       | 23.50        | .0        | .0        |          |

(1) UNITS: MG/L IN WATER COLUMN (L,H,B); G (D.W.)/SQUARE METER IN (B).
(2) DIMENSIONLESS NUMBERS.
(3) UNITS: CELLS/ML IN L, E, H; CELLS/100 G D.W. IN B.

Table 11 (continued)

TABLE 4. INPUT DATA DESCRIBING ENVIRONMENT: DEPTHS AND INFLOWS.

| # TY | DEPTH M | STFLO CU M/HR | STSED KG/HR | NPSFL CU M/HR | NPSED KG/HR | INTFL CU M/HR |
|------|---------|---------------|-------------|---------------|-------------|---------------|
| 1L | .1707 | 988.8 | 2.967 | | | 162.5 |
| 2B | 9.140E-03 | | | | | 1.626E-02 |
| 3L | .1798 | 46.94 | .4890 | | | |
| 4B | 9.140E-03 | | | | | |
| .3048 | 770.8 | 5.528 | | | | |
| 6R | 9.140E-03 | | | | 117.9 | 1.179E-02 |
| 7L | .3048 | | | | | 117.7 |
| 8B | 9.140E-03 | | | | | .1179 |
| 9L | .3048 | | | | | 117.7 |
| 10B | 9.140E-03 | | | | | .1533 |

Table 11 (continued)

TABLE 5.    INPUT DATA DESCRIBING ENVIRONMENT: SEDIMENT CHARACTERISTICS.

| # TY | SDCHR (1) | PCTWA (2) | FROC (3) | CEC (4) | AEC (4) | DOC MG/L |
|------|-----------|-----------|----------|---------|---------|----------|
| 1L   | 3.000     |           | 3.800E-02 | 25.00 | 25.00 | .0 |
| 2B   | 1.530     | 115.2     | 3.800E-02 | 25.00 | 25.00 |    |
| 3L   | 3.000     |           | 3.800E-02 | 25.00 | 25.00 | .0 |
| 4B   | 1.530     | 115.2     | 3.800E-02 | 25.00 | 25.00 |    |
| 5L   | 7.500     |           | 3.800E-02 | 25.00 | 25.00 | .0 |
| 6B   | 1.530     | 115.2     | 3.800E-02 | 25.00 | 25.00 |    |
| 7L   | 7.500     |           | 3.800E-02 | 25.00 | 25.00 | .0 |
| 8B   | 1.530     | 115.2     | 3.800E-02 | 25.00 | 25.00 |    |
| 9L   | 7.500     |           | 3.800E-02 | 25.00 | 25.00 | .0 |
| 10B  | 1.530     | 115.2     | 3.800E-02 | 25.00 | 25.00 |    |

(1) UNITS: MG/L SUSPENDED SEDIMENT IN L, E, H; BULK DENSITY (G/CC) IN B
(2) 100 * F.W./D.W. IN B.
(3) DIMENSIONLESS.
(4) MEQ/100 GRAMS DRY WEIGHT.

Table 11 (continued)

TABLE 6.  INPUT DATA DESCRIBING ENVIRONMENT: AERATION, LIGHT, MISC.

| # TY | KO2 CM/HR @20 | WIND M/S @10 CM | CMPET /M | DFAC M/M | EVAP MM/MON | AREA SQ M |
|---|---|---|---|---|---|---|
| 1L | .0 | .0 | 1.161 | .0 | .0 | 5.386E+04 |
| 2B | | | | | | 5.386E+04 |
| 3L | .0 | .0 | 1.161 | .0 | .0 | 1.257E+04 |
| 4B | | | | | | 1.257E+04 |
| 5L | .0 | .0 | 2.691 | .0 | .0 | 8.757E+04 |
| 6B | | | | | | 8.757E+04 |
| 7L | .0 | .0 | 2.691 | .0 | .0 | 8.757E+04 |
| 8B | | | | | | 8.757E+04 |
| 9L | .0 | .0 | 2.691 | .0 | .0 | 8.757E+04 |
| 10B | | | | | | 8.757E+04 |

Table 11 (continued)

TABLE 7. INPUT DATA DESCRIBING ENVIRONMENT: ADVECTIVE INTERCONNECTIONS.

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| COMP. NO. (JFRAD) | 1 | 3 | 5 | 7 | 9 |
| CONNECTED (ITOAD) | 3 | 5 | 7 | 9 | 0 |
| ADVECTION (ADVPR) | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| COMP. NO. (JFRAD) | 2 | 4 | 6 | 8 | 10 |
| CONNECTED (ITOAD) | 1 | 3 | 5 | 7 | 9 |
| ADVECTION (ADVPR) | .900 | .900 | .900 | .240 | .380 |
| COMP. NO. (JFRAD) | 2 | 4 | 6 | 8 | 10 |
| CONNECTED (ITOAD) | 4 | 6 | 8 | 10 | 0 |
| ADVECTION (ADVPR) | .100 | .100 | .100 | .760 | .620 |

TABLE 8. INPUT DATA DESCRIBING ENVIRONMENT: TURBULENT INTERCONNECTIONS.

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| OCOMP. NO. (JTURB) | 1 | 3 | 5 | 7 | 9 |
| CONNECTED (ITURB) | 2 | 4 | 6 | 8 | 10 |
| X-SECTION (XSTUR) | 5.39E+04 | 1.26E+04 | 8.76E+04 | 8.76E+04 | 8.76E+04 |
| CHAR. LN. (CHARL) | 8.99E-02 | 9.45E-02 | .157 | .157 | .157 |
| EUDY DISP. (DSP) | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 |

Table 12

EXAMS Output

TABLE 9. TRANSPORT PROFILE OF ECOSYSTEM.

| CP T* Y | VOLUME (CUBIC M) | SEDIMENT MASS (KG) | WATER FLOW (CU. M/DAY) | SED. FLOW (KG/DAY) | RESIDENCE TIME (DAYS) WATER | SEDIMENTS |
|---|---|---|---|---|---|---|
| 1L | 9.32E+03 | 27.9 | 2.76E+04 | 313. | .337 | 8.93E-02 |
| 2B | 495. | 6.58E+05 | 1.84 | 9.80E+03 | 54.3 | 67.1 |
| 3L | 3.35E+03 | 10.1 | 2.88E+04 | 114. | .117 | 8.85E-02 |
| 4B | 115. | 1.53E+05 | .361 | 2.15E+03 | 64.2 | 71.1 |
| 5L | 2.63E+04 | 198. | 5.01E+04 | 471. | .526 | .420 |
| 6B | 801. | 1.06E+06 | 1.64 | 9.08E+03 | 98.7 | 117. |
| 7L | 2.63E+04 | 198. | 5.29E+04 | 2.69E+03 | .498 | 7.34E-02 |
| 8B | 801. | 1.06E+06 | 4.21 | 2.32E+04 | 38.4 | 45.9 |
| 9L | 2.63E+04 | 198. | 5.57E+04 | 1.76E+03 | .473 | .112 |
| 10B | 801. | 1.06E+06 | 7.20 | 3.28E+04 | 22.4 | 32.5 |

* COMP. TYPE: "L"=LITTORAL; "E"=(EPI) AND "H"=(HYPO)LIMNION; "B"=BENTHIC

Table 12 (continued)

TABLE 10. KINETIC PROFILE OF ORGANIC TOXICANT. RATE CONSTANTS DERIVED
FROM COUPLING OF TOXICANT CHARACTERISTICS TO ECOSYSTEM PROPERTIES.

| CP T* | --------- PSEUDO-FIRST-ORDER RATE CONSTANTS (/HR) --------- | | | | | |
|-------|-----------|-----------|-----------|-----------|------------|-----------|
| Y | HYDROLYSIS | PHOTOLYSIS | OXIDATION | BIOLYSIS | VOLATILITY | TRANSPORT |
| 1L | .0 | .0 | .0 | .0 | .0 | .197 |
| 2B | .0 | .0 | .0 | .0 | .0 | 6.21E-04 |
| 3L | .0 | .0 | .0 | .0 | .0 | .369 |
| 4B | .0 | .0 | .0 | .0 | .0 | 5.86E-04 |
| 5L | .0 | .0 | .0 | .0 | .0 | 8.56E-02 |
| 6B | .0 | .0 | .0 | .0 | .0 | 3.56E-04 |
| 7L | .0 | .0 | .0 | .0 | .0 | .146 |
| 8B | .0 | .0 | .0 | .0 | .0 | 9.08E-04 |
| 9L | .0 | .0 | .0 | .0 | .0 | .133 |
| 10B | .0 | .0 | .0 | .0 | .0 | 1.28E-03 |

* COMP. TYPE: "L"=LITTORAL; "E"=(EPI) AND "H"=(HYPO)LIMNION; "B"=BENTHIC

Table 12 (continued)

TABLE 11.   CANONICAL PROFILE OF ECOSYSTEM.

| CP T* | PH | POH | TEMP DEG. C. | REAERATION COEFF. M/HR | COMPOSITE LIGHT % | BACTERIAL AVE POP. CELLS/** | SIZE % | OXIDANT CONC. (MOLAR) | DISSOLVED PERCENT % |
|-------|------|------|------|------|------|------|------|------|------|
| .0 | .0 | .0 | .0 | .0 | .0 | 1.00E-09 | 78.5 | | |
| 2B | 7.14 | 6.86 | 23.5 | .0 | .0 | .0 | .0 | .0 | 6.91E-03 |
| 3L | 7.01 | 6.99 | 23.5 | .0 | .0 | .0 | .0 | 1.00E-09 | 89.8 |
| 4B | 7.01 | 6.99 | 23.5 | .0 | .0 | .0 | .0 | 5.00E-10 | 3.11E-02 |
| 5L | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | .0 | 68.1 |
| 6B | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | 1.00E-09 | 2.28E-02 |
| 7L | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | 1.00E-09 | 87.2 |
| 8B | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | 5.00E-10 | 3.01E-03 |
| 9L | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | 1.00E-09 | 84.3 |
| 10B | 7.08 | 6.92 | 23.5 | .0 | .0 | .0 | .0 | .0 | 4.06E-03 |

* COMP. TYPE: "L"=LITTORAL; "E"=(EPI) AND "H"=(HYPO)LIMNION; "B"=BENTHIC
** ACTIVE BACTERIAL POPULATIONS AS CELLS/ML IN WATER COLUMN, CELLS/100 G (DRY WEIGHT) OF SEDIMENTS IN BOTTOM SEDIMENTS.

Table 12 (continued)

TABLE 12. TOXICANT LOADINGS (KG/HR) BY SYSTEM ELEMENT.

| ELEMENT | STREAM FLOW | RAINFALL | INTERFLOW | NPS LOAD | DRIFT LOAD |
|---|---|---|---|---|---|
| 1 | 1.284E-02 | | 6.505E-04 | | |
| 2 | | | | | |
| 3 | 4.404E-03 | | | | |
| 4 | | | | | |
| 5 | 3.361E-02 | | 1.179E-04 | | |
| 6 | | | 1.179E-04 | | |
| 7 | | | | | |
| 8 | | | 1.179E-04 | | |
| 9 | | | | | |
| 10 | | | 1.179E-04 | | |

Table 12 (continued)

TABLE 13. DISTRIBUTION OF CHEMICAL AT STEADY STATE: IN THE WATER COLUMN:

CUMP STEADY-STATE RESIDENT MASS  ********* TOXICANT CONCENTRATIONS *********
TU  2                             TOTAL   DISSOLVED SORBED BY SORBED BY PRECIP

| NTS | G/M | KILOS | % | MG/* | MG/L | BIOTA UG/G | SEDIMENTS MG/KG | SEDIME MG/ |
|---|---|---|---|---|---|---|---|---|
| 1 | 1.99E-03 | .1073 | 6.87 | 1.15E-02 | 9.05E-03 | .0 | 826. | .0 |
| 3 | 3.98E-03 | 5.005E-02 | 3.20 | 1.49E-02 | 1.34E-02 | .0 | 507. | .0 |
| 5 | 7.43E-03 | .6504 | 41.63 | 2.47E-02 | 1.68E-02 | .0 | 1.05E+03 | .0 |
| 7 | 4.84E-03 | .4235 | 27.10 | 1.61E-02 | 1.40E-02 | .0 | 274. | .0 |
| 9 | 3.78E-03 | .3311 | 21.19 | 1.26E-02 | 1.06E-02 | .0 | 263. | .0 |

SUBTOTAL: 1.562  1.90
AND IN THE BOTTOM SEDIMENTS:

| NTS | G/M | KILOS | % | MG/* | MG/L | BIOTA UG/G | SEDIMENTS MG/KG | SEDIME MG/ |
|---|---|---|---|---|---|---|---|---|
| 2 | .256 | 13.79 | 17.13 | 21.0 | 9.53E-03 | .0 | 21.0 | .0 |
| 4 | .109 | 1.370 | 1.70 | 8.98 | 1.84E-02 | .0 | 8.98 | .0 |
| 6 | .137 | 12.03 | 14.94 | 11.3 | 1.70E-02 | .0 | 11.3 | .0 |
| 8 | .332 | 29.10 | 36.14 | 27.4 | 5.42E-03 | .0 | 27.4 | .0 |
| 10 | .277 | 24.23 | 30.10 | 22.8 | 6.09E-03 | .0 | 22.8 | .0 |

SUBTOTAL: 80.53  98.10
TOTAL MASS (KILOGRAMS) = 82.09

Table 12 (continued)

TABLE 12. AVERAGE, MAXIMUM, AND MINIMUM CONCENTRATIONS AT STEADY STATE.

| [1] | CP)TOTAL | CP)DISSOLVED | CP)SEDIMENTS | CP)BIOTA | CP)PRECIP | CP)MASS |
|---|---|---|---|---|---|---|
| | MG/* | MG/L | MG/KG | UG/G | MG/L | G/M |
| **WATER COLUMN:** | | | | | | |
| AV | 1.60E-02 | 1.28E-02 | 584. | .0 | .0 | 4.4E-03 |
| MA | 5) 2.47E-02 | 5) 1.68E-02 | 5) 1.05E+03 | 9) .0 | 9) .0 | 5) 7.4E-03 |
| MI | 1) 1.15E-02 | 1) 9.05E-03 | 9) 263. | 9) .0 | 9) .0 | 1) 2.0E-03 |
| **BOTTOM SEDIMENTS:** | | | | | | |
| AV | 18.3 | 1.13E-02 | 18.3 | .0 | .0 | .22 |
| MA | 3) 27.4 | 4) 1.84E-02 | 8) 27.4 | 10) .0 | 10) .0 | 8) .33 |
| MI | 4) 8.98 | 3) 5.42E-03 | 4) 8.98 | 10) .0 | 10) .0 | 4) .11 |

1 NUMBER IN HALF-PARENS (CP) INDICATES COMPARTMENT WHERE VALUE WAS FOUND.
* TOTAL CONCENTRATION AS MG/L IN WATER COLUMN, AS MG/KG IN SEDIMENTS.

sediments), the average, maximum and minimum concentra-
tions at steady state. Table 10, the kinetic profile is
for organic toxicants only. These five tables are
repeated the number of times EXAMS uses MINTEQ to update
steady state metal concentrations. For the Naugatuck
River test case, this occurred three times. The most
important of the three outputs is the last repetition,
because it is the output obtained when system steady
state has been achieved for the water column and sedi-
ments.

The third section of output is encompassed in
Table 15 - 17, the analysis of steady state fate, the
simulation of system response after load ceases, and the
exposure analysis summary. These three tables contain the
persistence calculation performed by EXAMS. These tables
are presented in Table 13. The final portion of the
program output is the MISP output.

## 3.5 Output (MISP)

This section as previously stated provides a
summary of the EXAMS-MINTEQ interactions. These interac-
tions include steady state calculations made to achieve
system steady state, and calculations made during the
persistence to update metal fractions. For the Naugatuck
River test case, steady state concentrations were updated
three times to obtain system equilibrium, and updated

Table 13

EXAMS Output

CHEMICAL: Heavy Metal
ECOSYSTEM: NAUGATUCK RIVER CALIBRATION TEST RUN

TABLE 15.   ANALYSIS OF STEADY-STATE FATE OF ORGANIC TOXICANT.

| PROCESS | MASS FLUX KG/DAY | % OF LOAD | HALF-LIFE* DAYS |
|---|---|---|---|
| HYDROLYSIS | .0 | 0.0 | -- |
| OXIDATION | .0 | 0.0 | -- |
| PHOTOLYSIS | .0 | 0.0 | -- |
| ALL CHEMICAL PROCESSES | .0 | 0.0 | -- |
| WATER COLUMN (BACTERIA) | .0 | 0.0 | -- |
| BOTTOM SEDIMENTS (BACTERIA) | .0 | 0.0 | -- |
| TOTAL BIOLYSIS | .0 | 0.0 | -- |
| VOLATILIZATION | .0 | 0.0 | -- |
| WATER-BORNE EXPORT | 1.245 | 100.00 | 45.72 |
| TRANSFORMATION AND TRANSPORT | 1.245 | 100.00 | |
| TOTAL SYSTEM LOAD | 1.245 | | |
| RESIDUAL ACCUMULATION RATE: | 1.341E-06 | 0.00 | |

* HALF-LIVES ARE ESTIMATES BASED ON A FIRST-ORDER RATE APPROXIMATION.

Table 13 (continued)

CHEMICAL: Heavy Metal
ECOSYSTEM: NAUGATUCK RIVER CALIBRATION TEST RUN

TABLE 16. SIMULATION OF SYSTEM RESPONSE AFTER LOAD CEASES.

| TIME | AVERAGE POLLUTANT CONCENTRATIONS | | | | MASS OF POLLUTANT | |
|---|---|---|---|---|---|---|
| | WATER COLUMN | | BOTTOM SEDIMENTS | | WATER COL | SEDIMENTS |
| DAYS | FREE(MG/L) | SED(MG/KG) | PORE(MG/L) | SED(MG/KG) | TOTAL KG | TOTAL KG |
| 0. | 1.28E-02 | 584. | 1.13E-02 | 18.3 | 1.562 | 80.5 |
| 8. | 3.75E-03 | 165. | 1.06E-02 | 17.0 | .4264 | 74.5 |
| 16. | 3.46E-03 | 153. | 9.91E-03 | 15.6 | .3934 | 68.4 |
| 24. | 3.20E-03 | 142. | 9.26E-03 | 14.4 | .3630 | 62.7 |

Table 13 (continued)

TABLE 17.  EXPOSURE ANALYSIS SUMMARY.
-------------------------------------

EXPOSURE:
A. MAXIMUM CONC. IN WATER COLUMN: 1.7E-02 MG/L DISSOLVED, 2.5E-02 TOT
   MAX. CONC. IN BOTTOM SEDIMENT: 1.8E-02 MG/L DISSOLVED IN PORE WATER
B. BIOSORPTION - MAX. CONCENTRATION - PLANKTON: .0     UG/G
                                        BENTHOS: .0     UG/G

C. MAXIMUM TOT. CONC. IN SEDIMENT DEPOSITS: 27.   MG/KG (DRY WEIGHT)

FATE:
A. TOTAL STEADY-STATE ACCUMULATION: 82.    KG; 1.90% IN WATER COL.,
   98.10% IN BOTTOM SEDIMENTS.

B. TOTAL LOAD: 1.2    KG/DAY - DISPOSITION:    0.0 % VIA CHEMICAL
   TRANSFORMATIONS,    0.0 % BIOTRANSFORMED,    0.0 % VOLATILIZED,
   100.00% EXPORTED VIA OTHER PATHWAYS.

PERSISTENCE:
A. AT THE END OF A  96.0   DAY RECOVERY PERIOD, THE WATER COLUMN HAD
   LOST 76.77% OF ITS INITIAL TOXICANT BURDEN; THE SEDIMENTS HAD
   LOST 22.16% OF THEIR INITIAL BURDEN ( 23.20% REMOVAL OVERALL).
B. SYSTEM SELF-PURIFICATION TIME IS ROUGHLY******** YEARS.

| | | | | | | |
|---|---|---|---|---|---|---|
| 32. | 2.96E-03 | 131. | 8.67E-03 | 13.2 | .3352 | 57.4 |
| 40. | 2.74E-03 | 122. | 8.10E-03 | 12.2 | .3094 | 52.6 |
| 48. | 2.53E-03 | 113. | 7.57E-03 | 11.2 | .2857 | 48.2 |
| 56. | 2.34E-03 | 105. | 7.07E-03 | 10.3 | .2638 | 44.2 |
| 64. | 2.16E-03 | 97.1 | 6.60E-03 | 9.46 | .2436 | 40.5 |
| 72. | 2.00E-03 | 90.0 | 6.17E-03 | 8.71 | .2252 | 37.2 |
| 80. | 1.85E-03 | 83.5 | 5.76E-03 | 8.02 | .2082 | 34.1 |
| 88. | 1.71E-03 | 77.5 | 5.38E-03 | 7.39 | .1926 | 31.3 |

again two times during the persistence calculation. This
totals five interactions between EXAMS and MINTEQ, and
the MISP output file is presented in Table 14.

Table 14

MISP Output

```
UPDATED CONCENTRATIONS FROM MINTEQ (MG/L)
UPDATED CONCENTRATIONS FROM MINTEQ (MG/L)
COMPARTMENT      AQUEOUS     ADSORBED    PRECIPITATED
COMPARTMENT      AQUEOUS     ADSORBED    PRECIPITATED
          1    9.024E-03   2.478E-03    0.0
          2    9.532E-03   1.379E+02    0.0
          3    1.341E-02   1.519E-03    0.0
          4    1.836E-02   5.897E+01    0.0
          5    1.684E-02   7.880E-03    0.0
          6    1.697E-02   7.435E+01    0.0
          7    1.404E-02   2.065E-03    0.0
          8    5.420E-03   1.798E+02    0.0
          9    1.061E-02   1.970E-03    0.0
         10    6.094E-03   1.500E+02    0.0
CONCENTRATIONS COMPUTED BY EXAMS IN MG/L
CONCENTRATIONS COMPUTED BY EXAMS IN MG/L
```

# CHAPTER 4

## MODEL RESULTS

### 4.1 Calibration Parameters

Metal transport in the Naugatuck River is currently being investigated to provide important data for waste allocation decisions. Included within this investigation is the calibration of MEXAMS to a compartmentalized river reach. The reach being calibrated (Figure 3) was originally composed of three water column compartments and three benthic compartments. However, the final model configuration consisted of a ten compartment model; five benthic compartments and five water column compartments. A diagram of the final configuration will be presented herein. This calibration consisted of adjusting certain model inputs to yield results that were the same as the field data obtained on August 16-18, 1983.

The first step in the calibration was to determine which model inputs have the least reliability. These are the parameters that will be adjusted to perform a sensitivity analysis. Any sensitivity analysis is system dependent because certain input parameters may be more or less sensitive depending on the system being modeled.

Therefore, the first decision to be made was to select a system configuration. There are many possible configurations due to the possible advective and dispersive pathways. The two initial configurations chosen for this test case are presented in Figure 5. The main difference between configuration one and configuration two is the advective pathways. Configuration one allows flow to exit the system through the sediments via compartment six and has no advective flow through compartment four, configuration two is just the opposite. Originally, both of these configurations had the entire groundflow routed through the benthic compartments (2 & 6). This caused a considerable problem because the sediment residence time within the benthic compartments was so low that the priority pollutant was being flushed out of the system. This problem was corrected by routing a portion of the groundwater into the water column compartments (1 & 5). This increased the sediment residence time and thus, increased the concentration of adsorbed pollutant within the bed sediments. Figure 6 displays the effect of routing various percentages of groundwater through the benthic compartments for both configurations. Compartments two and four were not shown in configuration one because the residence time changed very little. This slight change is a result of no flow being advected through these compartments. On the other hand, compartment six is

# CALIBRATION CONFIGURATIONS

## CONFIGURATION 1
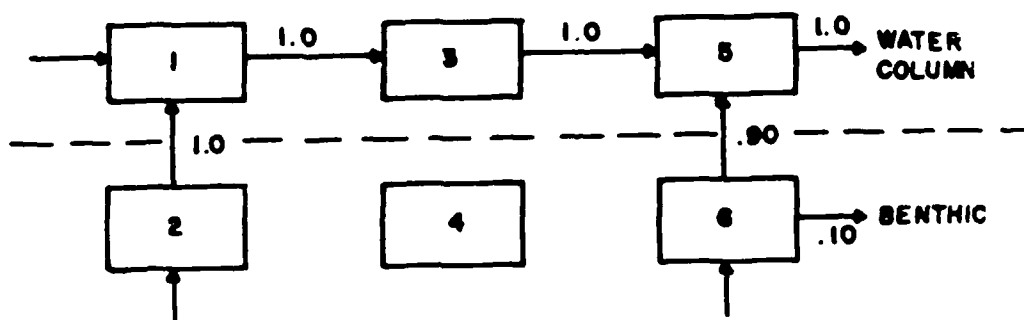


## CONFIGURATION 2
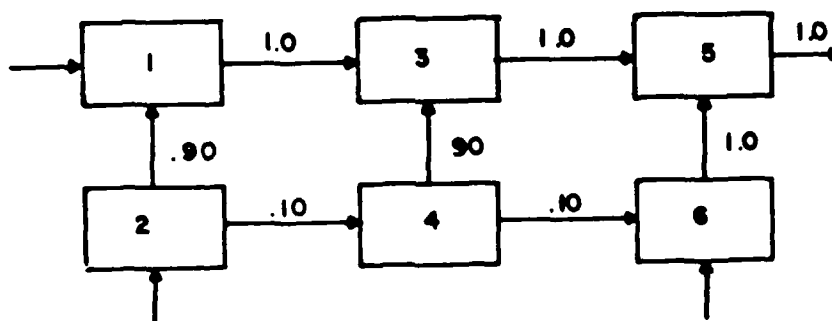


KEY: I-COMPARTMENT #'s
1.0-ADVECTIVE PROPORTION

Figure 5.

EFFECT OF GROUNDWATER ROUTING
ON SEDIMENT RESIDENCE TIMES
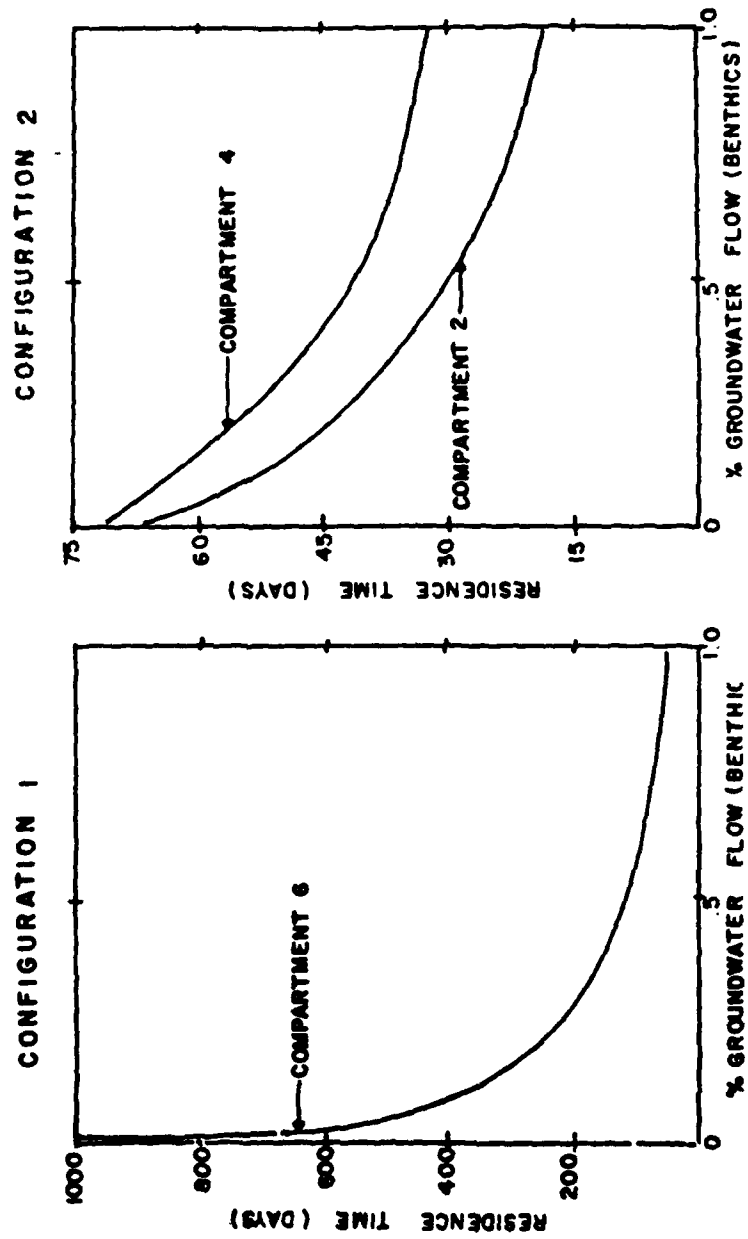


Figure 6.

not shown for configuration two because it also had very little change. Again, this is a result of no flow being advected through compartment six. At this point a decision was made to perform the remaining sensitivity analysis and calibration on configuration two.

The effect of the percent groundwater flow into the benthic compartments for configuration two allowed adjustment of the particulate concentration in the benthic regions (Figure 7). The next parameter adjusted for configuration two was the dispersion coefficient. This parameter was adjusted from 5.00*E-05 to 5.00*E-08 (meters square/hr) to obtain the relationship between dispersion coefficient and adsorbed concentration in the benthic compartments (Figure 8). The above range for dispersion coefficients did not result from a calculation because the slope of the river bed, the magnitude of the diffusive exchange coefficients for the water column and the interstitial water, and the characteristic length of the gradient were not known. However, a range of possible dispersion coefficients was obtained from Analysis of Fate of Chemicals in Receiving Waters - Phase I (1981, DiToro and St. John).

The trend shown by varying the dispersion coefficient resulted in the sensitivity analysis of a final parameter. This parameter was the $K_d$ and originally it was not to be a calibration variable. The reason behind

**EFFECT OF GROUNDWATER ROUTING ON
SEDIMENT CONCENTRATION IN BENTHIC COMPARTMENTS**
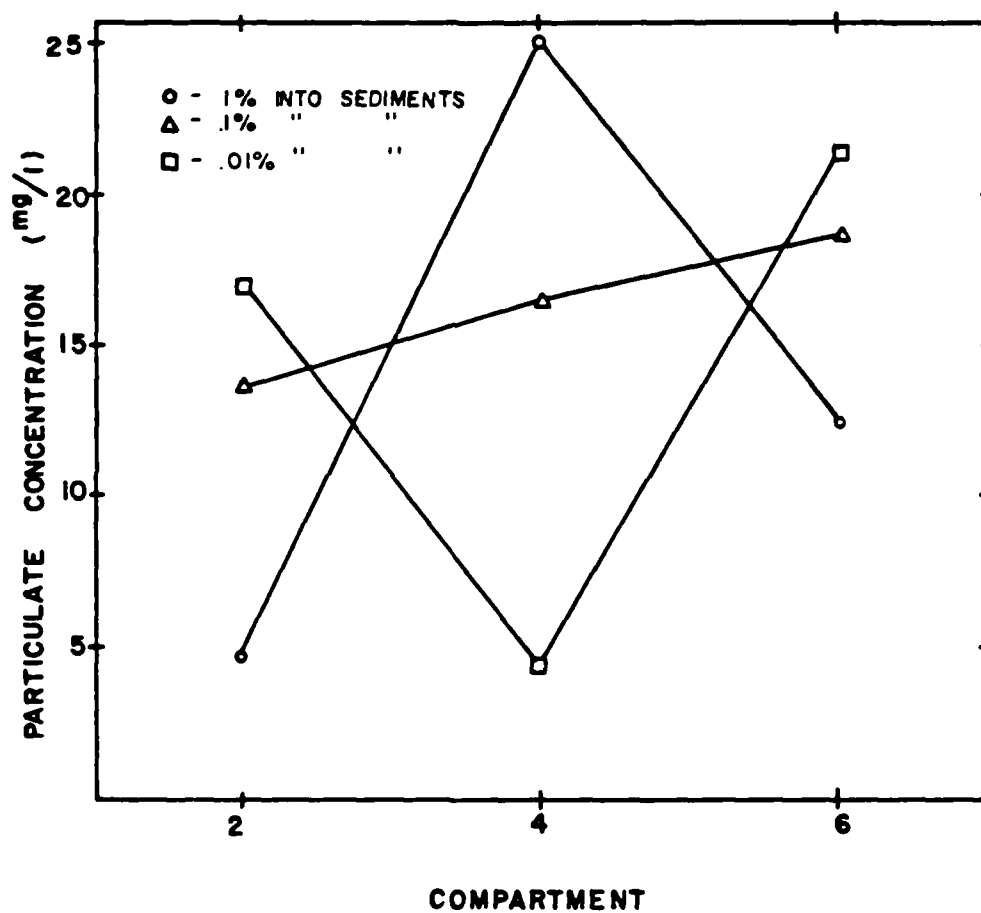


Figure 7.

DISPERSION  COEFFICIENT  VS.  CONCENTRATION
IN  BENTHIC  COMPARTMENTS
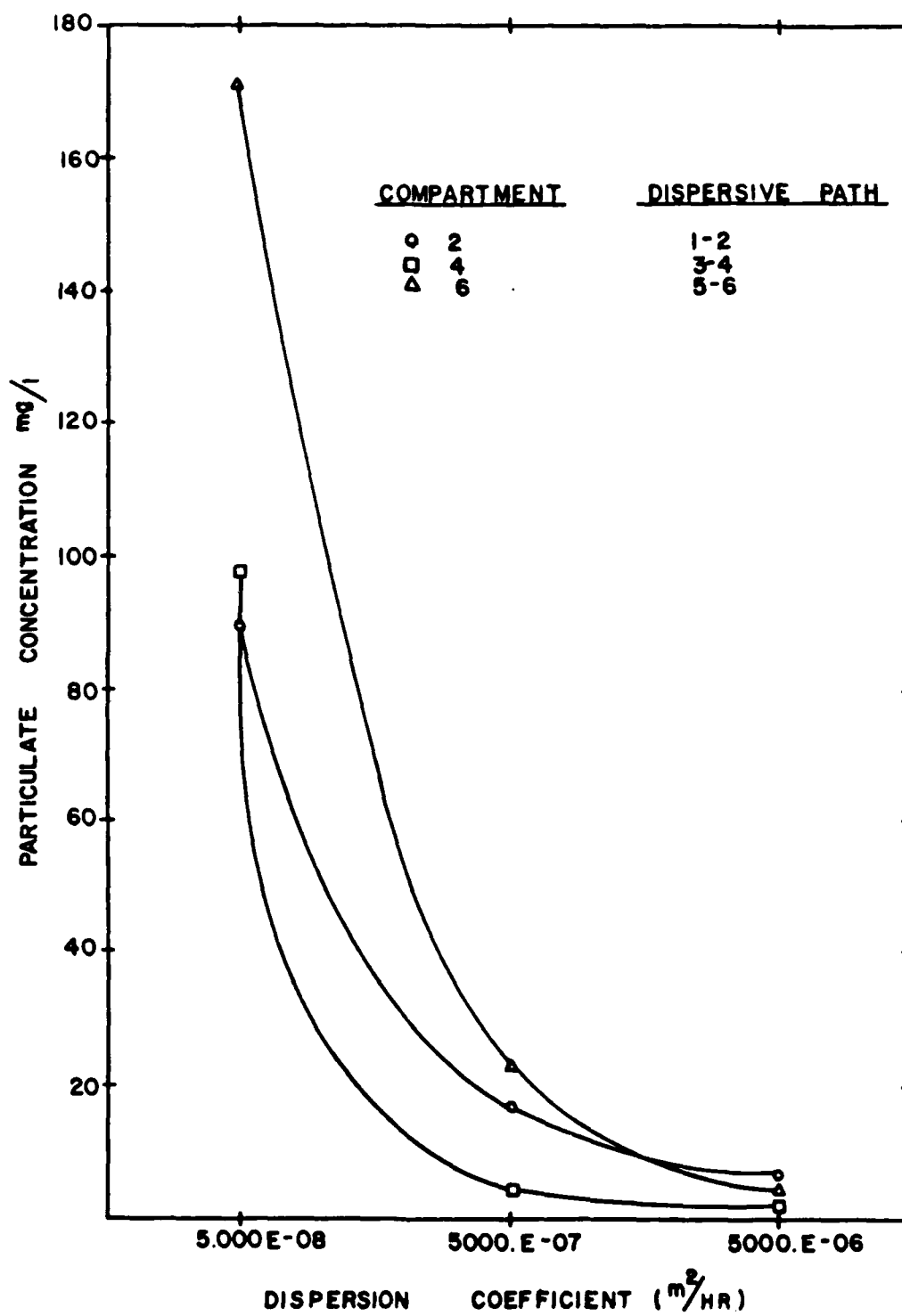


Figure 8.

the change stemmed from the inability to achieve the
required adsorbed concentration within the benthic com-
partments. The decision to increase the $K_d$ values from
their field-determined values was reasonable considering
the accuracy of benthic $K_d$ determinations made in the
field. It is very difficult to obtain a sediment sample
without entrainment of water from the water column. The
aqueous concentration of contaminant within the water
column is much lower than that within the bed sediments,
and the result would be a dilution. This dilution would
result in a $K_d$ value that was too low, and for this
reason the $K_d$ parameter has been changed to achieve
higher particulate concentrations within the bed sedi-
ments. The adjustment of the $K_d$ value and its affect on
the benthic compartment adsorbed concentrations are shown
in Figure 9.

Another problem was encountered after the
calibration of configuration two which resulted in a
final adjustment of the advective pathways. The problem
was that the total concentration in compartment five was
too high, and to reduce this an advective pathway from
the benthic compartment (compartment six) was es-
tablished. The advective flow proportions from compart-
ment six to compartment five were varied in effort to
reduce the total concentration in compartment five. The
results obtained from varying the advective flow are
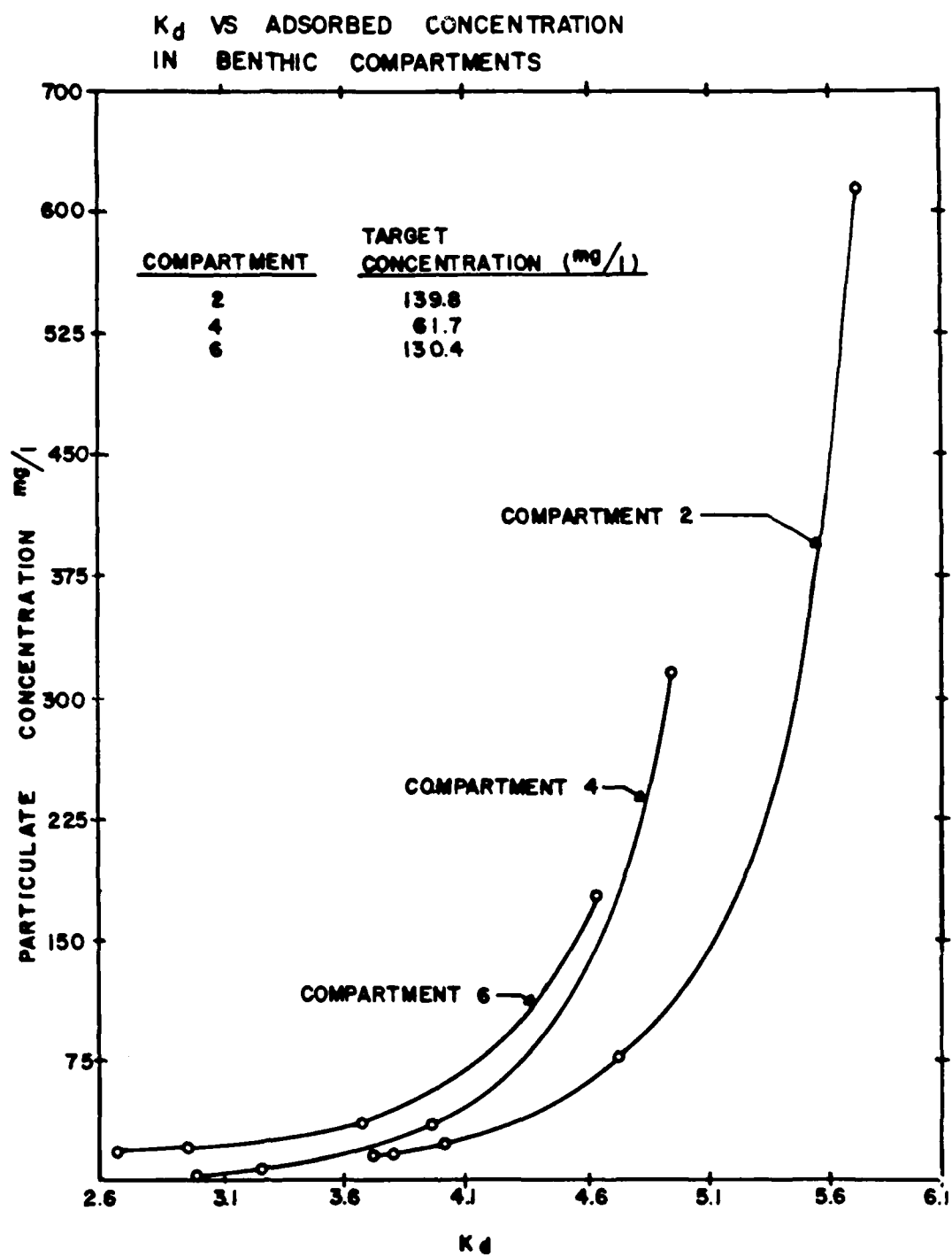
Figure 9.

presented in Figure 10.

The required concentrations for compartment five could not be obtained by varying the advective flow. As a result, a ten compartment configuration was developed. Since the model establishes instantaneous equilibrium, the 6.7 mile compartment was to large and the concentration could not be lowered by adjusting any of the calibration parameters. The final ten compartment configuration is presented in Figure 11. The final configuration was calibrated by adjusting three variables; the percent ground water flow into the benthic compartments (8 & 10), the advective flow between compartments (8 to 7, and 10 to 9), and the $K_d$ value for the benthic compartments.

## 4.2 Model Results

After a good understanding was achieved for the sensitivity of the calibration parameters, the calibration continued for the ten compartment model. The two models being compared are slightly different, because the incremental flow model utilizes point source loads as incremental loadings to the an existing concentration. This new concentration is then transported downstream. On the other hand, the MEXAMS model establishes instantaneous equilibrium with the point source load, and as a result, the model outputs are mean compartment outputs

EFFECT OF ADVECTIVE FLOW
FROM COMPARTMENT 6 TO COMPARTMENT 5
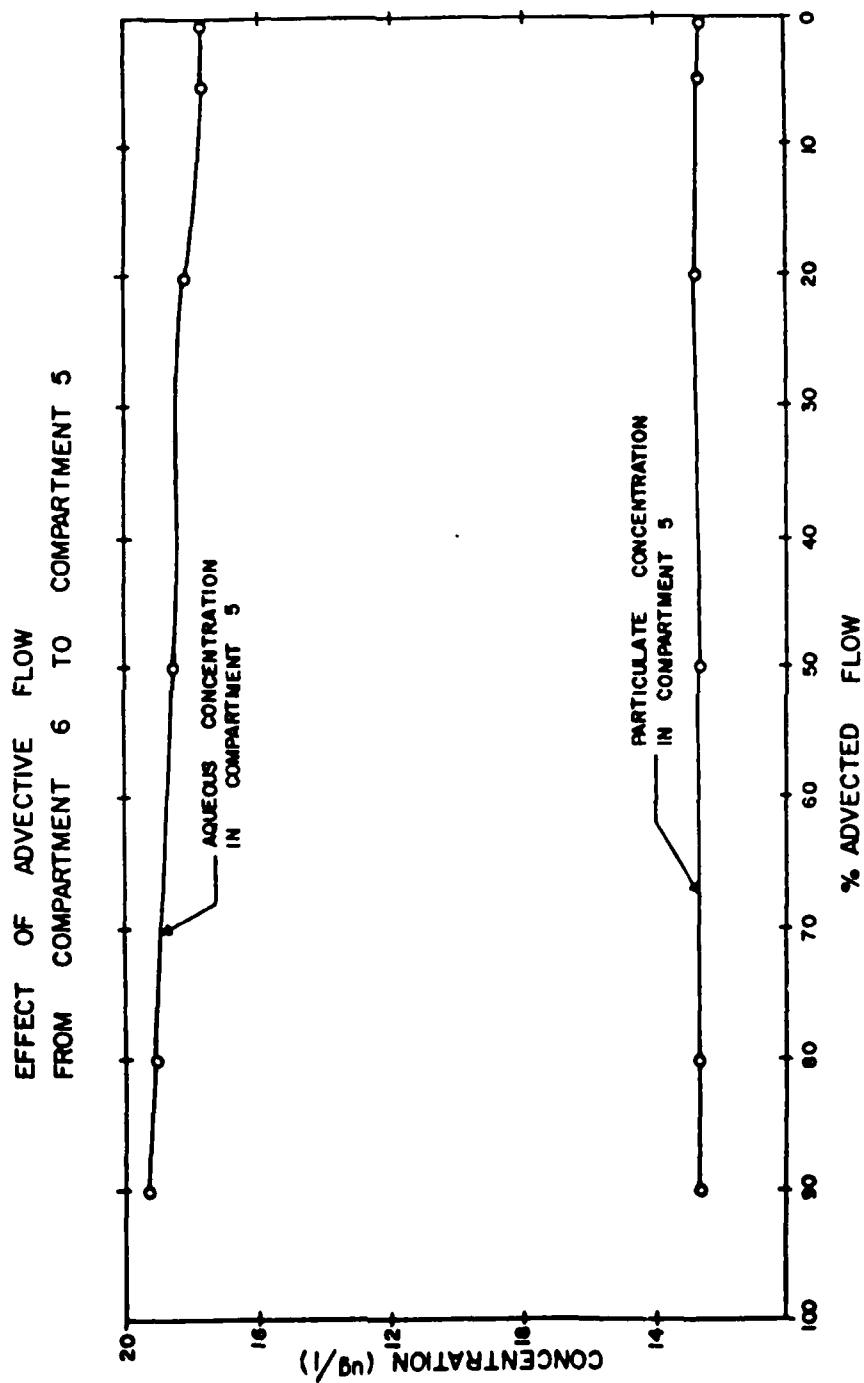
Figure 10.

FINAL CALIBRATION CONFIGURATION
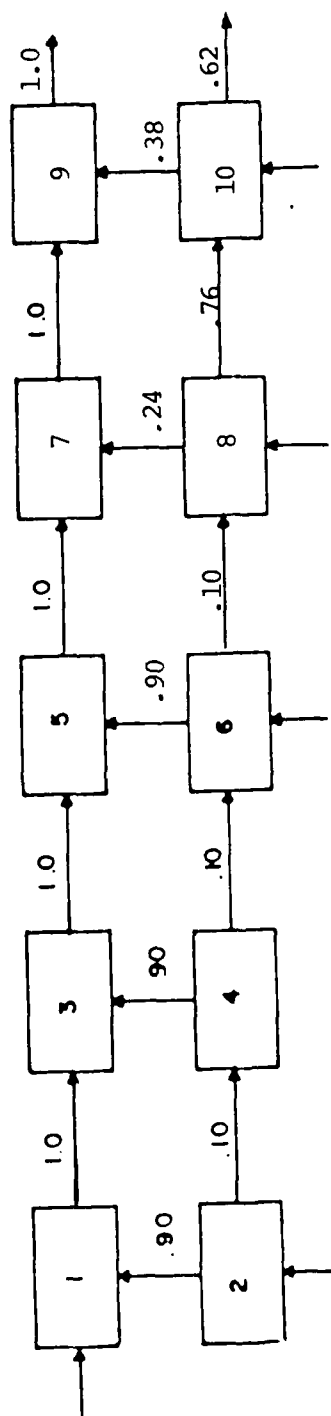


KEY: 1 - COMPARTMENT #'s
10 - ADVECTIVE PROPORTION

Figure 11.

and not outputs at various points within the r

Thus, the MEXAMS model will not predict the cc

where a point load enters (Bogue Rd.), and the

tion measured will be higher than predicted. 7

calibration was compared to an incremental flc

Curtis, State of Connecticut, Dept. of Enviror

Protection, and laboratory results obtained fr

collected at various sites along the river. Th

compartment model calibration to particulate c

tions within the benthic compartments was very

The model calibration to aqueous concentratior

the water column was not as accurate because c

five concentration were too high. As a result,

compartment was further divided into smaller c

ments. The six compartment model results are p

Figure 12 and Table 15.

This model was improved by dividing th

river segment into smaller compartments. The c

talization of compartments five and six into s

compartments would allow for a greater control

model calibration. The third segment has been

figured by splitting compartments five and si>

The calibration results obtained from the fine

figuration are presented in Figure 13 and Tab

respectively. As stated previously, three par

adjusted to achieve a calibrated model. Table

MODEL    CALIBRATION    RESULTS
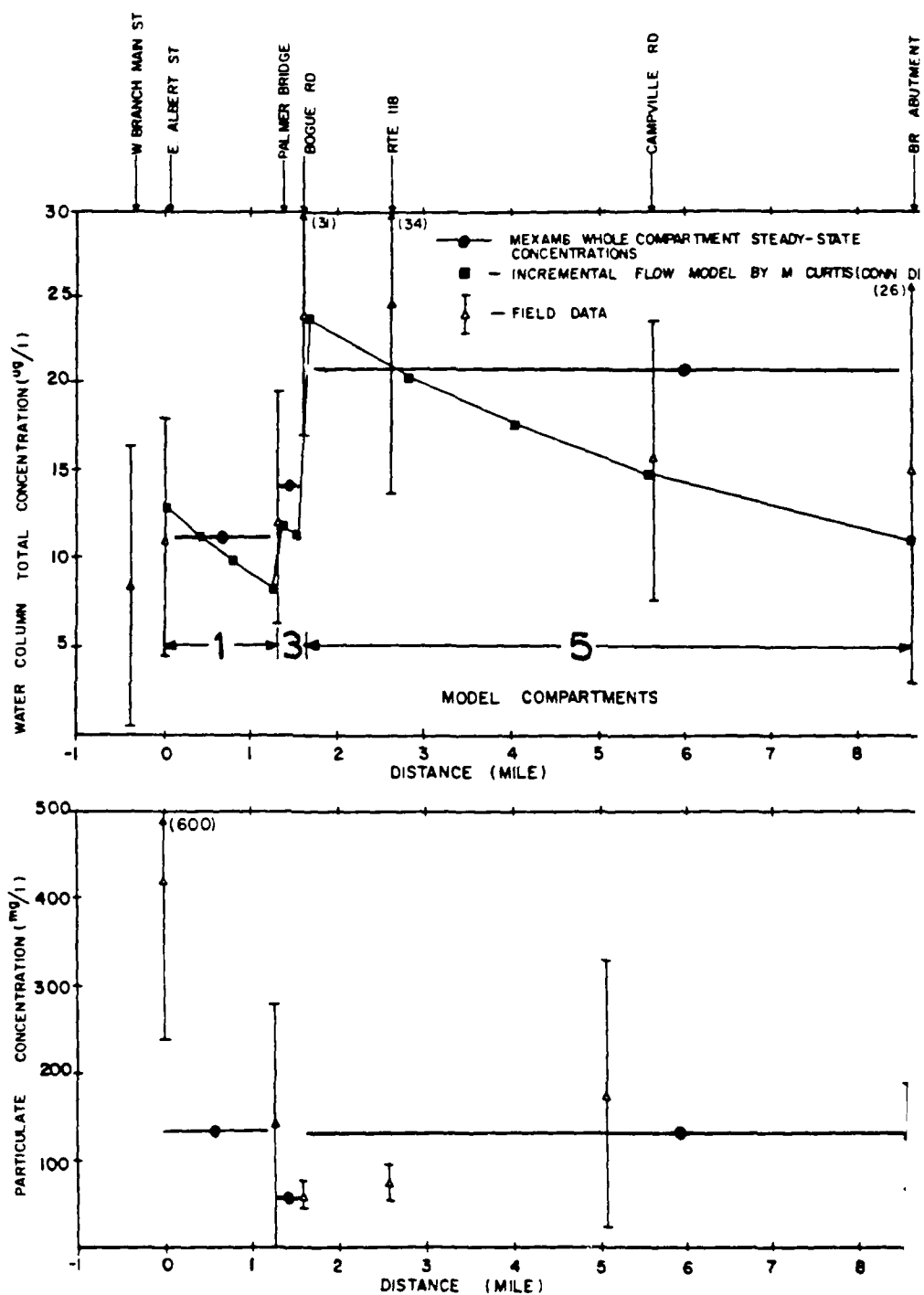


Figure 12.

Table 15

MODEL RESULTS FOR CONFIGURATION 3

| Location | Model Compartment | Total | | | Dissolved * | | |
|---|---|---|---|---|---|---|---|
| | | Field | Model | % Diff. | Field | Model | % Diff. |
| WATER COLUMN ( μg/1) | | | | | | | |
| Palmer Br. Rd. | 1 | 12. | 11.5 | -4.1 | 9.5 | 9.1 | -4.7 |
| Bogue Rd | 3 | ------No Segment Data------ | | | ------No Segment Data------ | | |
| Rte. 118 | | | | | | | |
| Campville Rd. } | 5 | 18.3 | 20.3 | +10.9 | 14.3 | 17.7 | +23.7 |
| Br. Abutment } | | | | | | | |
| BENTHIC REGION ( mg/1) | | | | | Particulate | | |
| Palmer Br. Rd. | 2 | 140. | 138. | -1.5 | 140. | 138. | -1.5 |
| Bogue Rd. | 4 | 62. | 59. | -4.8 | 62. | 59. | -5.0 |
| Rte. 118 | | | | | | | |
| Campville Rd. } | 6 | 128. | 133. | +3.5 | 127. | 133. | +4.7 |
| Br. Abutment } | | | | | | | |

* The benthic region is shown as particulate copper in mg/1

# MODEL CALIBRATION RESULTS
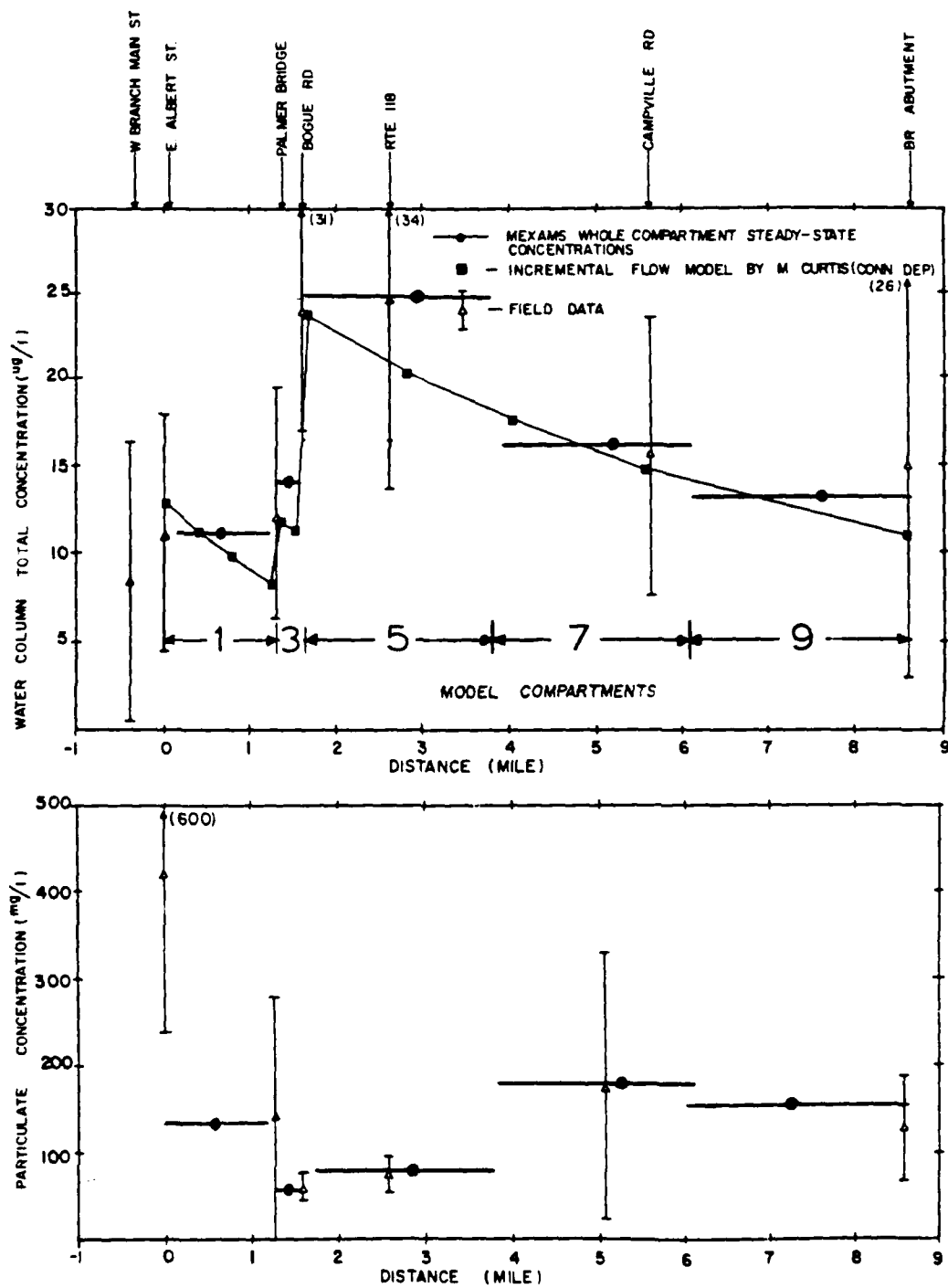


Figure 13.

Table 16

MEXAMS - NAUGATUCK RIVER MODEL RESULTS

| LOCATION | MODEL COMPARTMENT | TOTAL COPPER | | | DISSOLVED COPPER | | |
|---|---|---|---|---|---|---|---|
| | | FIELD | MODEL | % DIFF. | FIELD | MODEL | % DIFF. |
| WATER COLUMN ( g/l) | | | | | | | |
| Palmer Br. Rd. | 1 | 12. | 11.5 | -4.1 | 9.5 | 9.1 | -4.7 |
| Bogue Rd. | 3 | -----No Segment Data----- | | | -----No Segment Data----- | | |
| Rte. 118 | 5 | 24. | 24.6 | +2.5 | 17. | 16.8 | -1.2 |
| Campville Rd. | 7 | 16. | 16.6 | +3.8 | 14. | 14. | 0.0 |
| Br. Abutment | 9 | 14. | 12.6 | -10.0 | 11. | 10.6 | 3.6 |
| | | | | | PARTICULATE COPPER | | |
| BENTHIC REGION ( g/l) | | | | | | | |
| Palmer Br. Rd. | 2 | 140. | 138. | -1.5 | 140. | 138. | -1.5 |
| Bogue Rd. | 4 | 62. | 59. | -4.8 | 62. | 59. | -5.0 |
| Rte. 118 | 6 | 73. | 74. | +1.4 | 72. | 73. | +1.4 |
| Campville Rd. | 8 | 177. | 179. | +1.1 | 176. | 178. | +0.6 |
| Br. Abutment and Campville Rd. | 10 | 154.* | 150. | -2.6 | 154.* | 150. | -2.6 |

* The average copper concentration measured at Campville Rd. and the Bridge Abutment was used for comparison (based on model compartmentalization).

Table 17

Comparative Kd Data

| Compartment # | Original log Kd | Calibrated log Kd |
|:---:|:---:|:---:|
| 1 | 0.30 | 0.30 |
| 2 | 3.72 | 5.02 |
| 3 | -0.25 | -0.25 |
| 4 | 2.95 | 4.20 |
| 5 | -0.05 | -0.05 |
| 6 | 2.67 | 4.42 |
| 7 | -0.05 | -0.05 |
| 8 | 2.67 | 5.30 |
| 9 | -0.05 | -0.05 |
| 10 | 2.67 | 5.17 |

the original log $K_d$'s and the final log $K_d$'s used to
obtain the ten compartment calibration. The advective
flow paths for the new compartmentalizations were
presented in Figure 11, and the percent ground water
routed into benthic compartments eight and ten were
changed from .01% to .1% and .13%, respectively. The
final calibration for the ten compartment model was very
accurate, and the concentrations predicted by the model
were well within the error bars of the field data.

## 4.3 Future Loadings

Since the purpose of this report is to illustrate
the usefulness of the modeling system, the effect of an
increase in metal loading to compartment one was simu-
lated. This increase could be an additional discharger at
some point in the future, or an increase in production by
an existing discharger. The existing contaminant loading
is 1.284 E-02 $K_d$/hr and this was increased to 1.284 E-01
and 1.284 E+00. The effect of this increased metal load-
ing on both water column and benthic compartments is
displayed in Figure 14. This model, however, has some
limitations, and they will be discussed next, along with
recommendations for solving these drawbacks.

## 4.4 Limitations and Recommendations

The first limitation encountered dealt with the

EFFECTS OF SIMULATED INCREASED
METAL LOADINGS TO COMPARTMENT 1
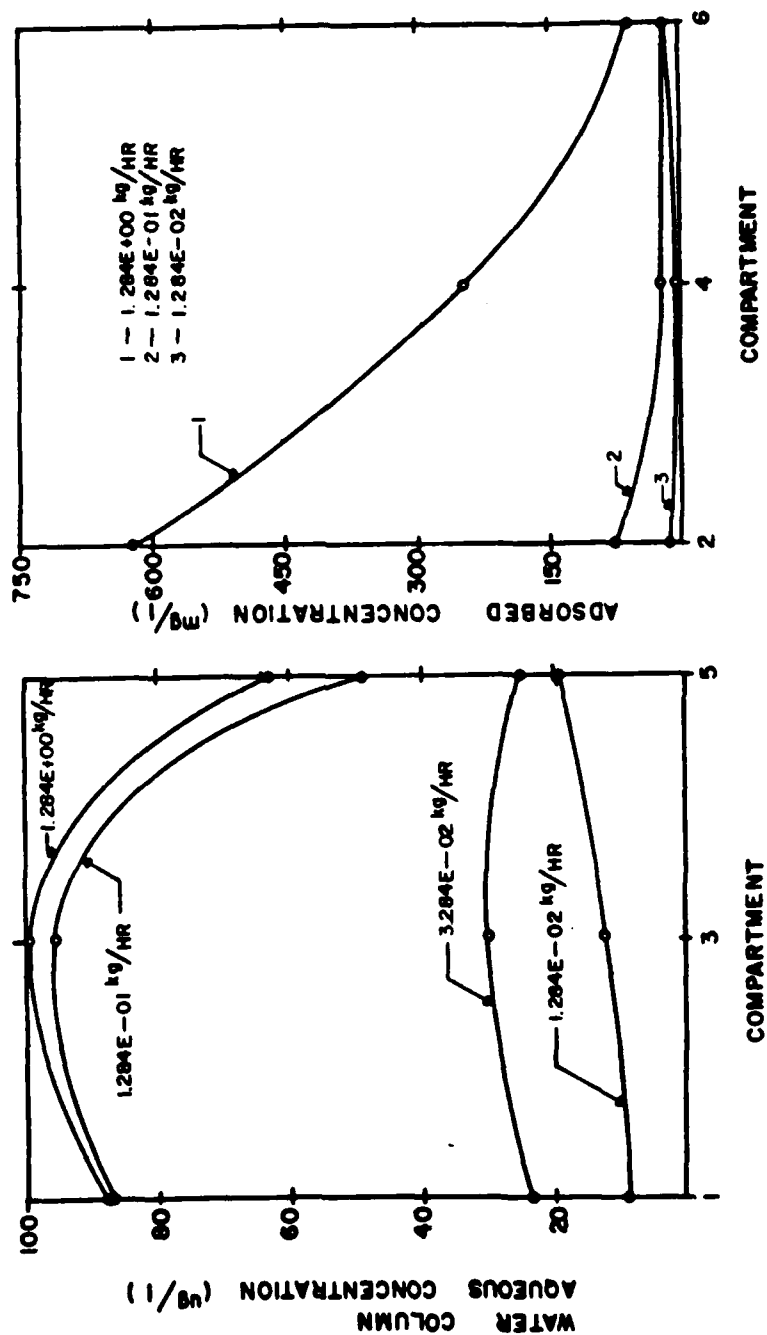
Figure 14.

availability of organic complexes within the thermodynamic data base of MINTEQ. MINTEQ had only a few fulvate and humate complexes. To alleviate this limitation, organic complexes with EDTA were added. A plot was obtained by varying the EDTA concentration. This graph is presented in Figure 15, and the effect of organic complexation with EDTA for three pollutant metals is displayed.

Another limitation to the model occurs during the persistence calculation. The program calculates how long it would take to purify the riverine system, which is incorrect and should instead calculate the time required to achieve a certain concentration. This concentration could correspond to a toxic level for a certain aquatic specie, or a desired concentration level, as required by some regulatory agency. This problem can be solved very easily by including an input parameter in the MISP input file. This parameter would correspond to the final concentration desired by the programmer (concentration due to upstream loadings).

To simulate concentrations within the water column prior to pollutant loadings, the point source chemical loads were removed and the model was utilized to obtain concentrations due to upstream loadings only. A comparison of the model results is presented in Figure 16.

# EFFECT OF COMPLEXING ORGANIC UPON ADSORPTION IN COMPARTMENT I.

LEGEND:

o — COPPER
△ — ZINC
□ — LEAD

$C_p$ $(ug/l)$

10

8

6

4

2

0 .1 .2 .3 .4

EDTA $(mg/l)$

Figure 15

TOTAL CONCENTRATION VS DISTANCE IN WATER COLUMN
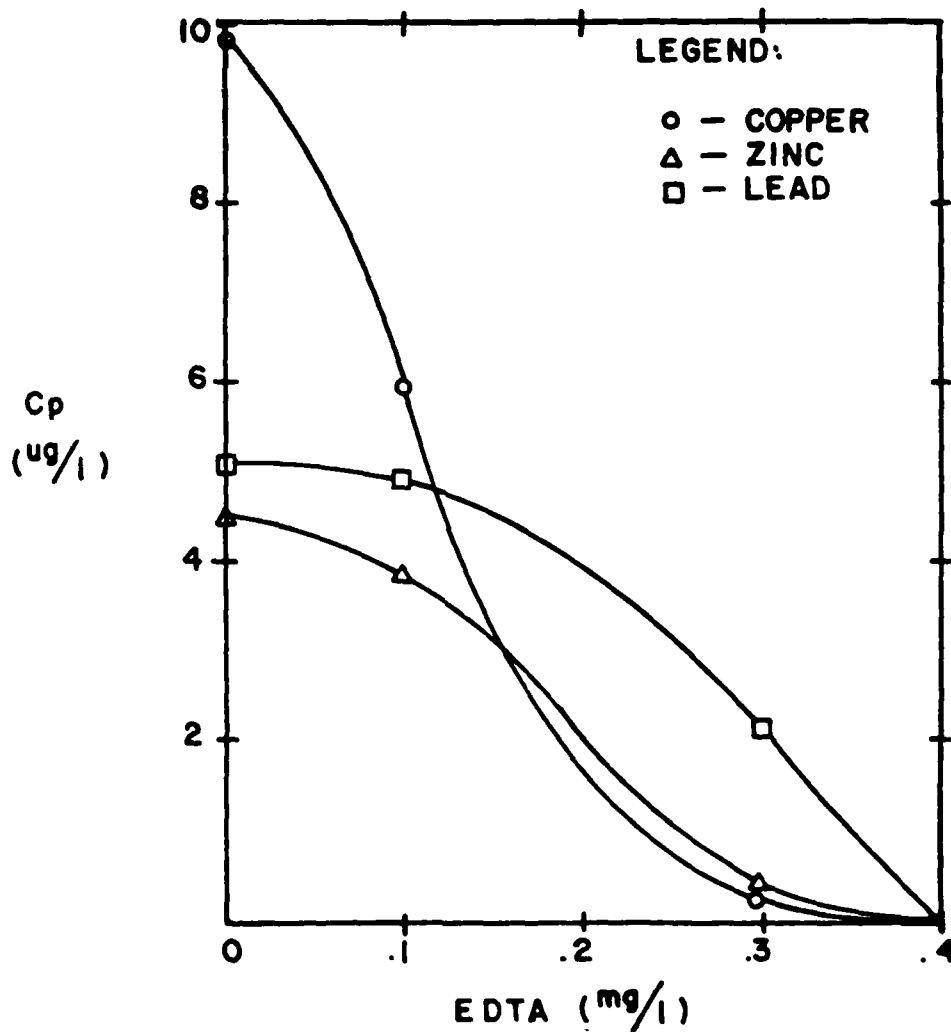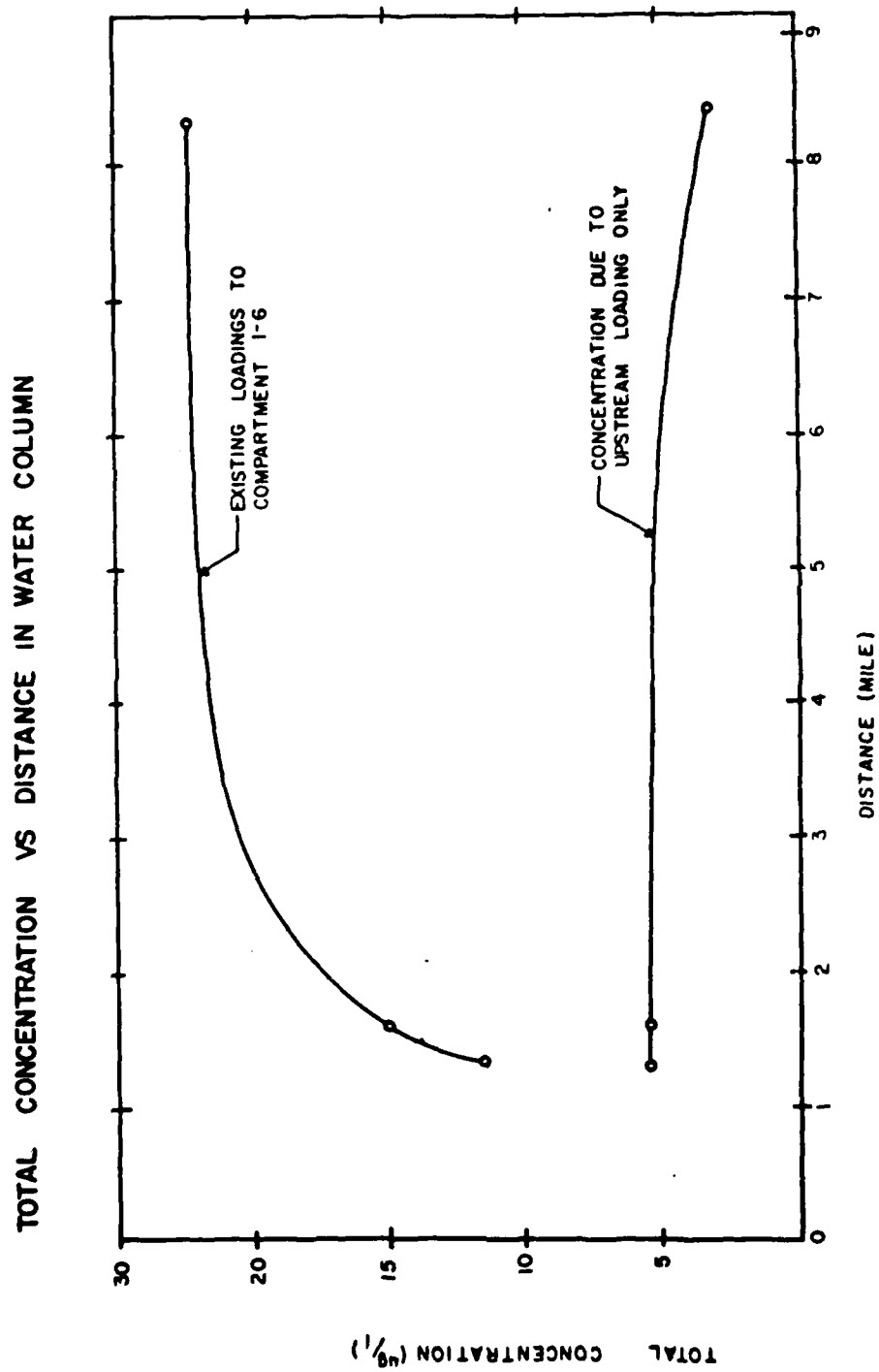
Figure 16

Other limitations include the ability to only run the program with one metal. This allows no competition and is unrealistic for an aquatic ecosystem.. Also, on the subject of competition, when using the $K_d$ "activity" approach, unlimited surface sites are assumed which is unrealistic. It is recommended that an input be established that would limit surface sites and make the model more realistic.

CHAPTER 5

CONCLUSIONS

The behavior of total, dissolved and particulate
(adsorbed copper within an 8.3 mile reach of the
Naugatuck River (East Albert St. to Thomaston Bridge
Abutment) was modeled using the Metals Exposure Assess-
ment Modeling System (MEXAMS). Data provided by the
Department of environmental Protection, State of Connec-
ticut concerning mass metal loading, system physical and
chemical characteristics was used to calibrate the MEXAMS
computer model for this test case.

The most important aspect of this model calibra-
tion was the compartmentalization (configuration) of the
river reach. The model was initially calibrated for a six
compartment configuration. However, the six compartment
configuration did not predict adequately (within 10%
error) the total and dissolved concentrations in the
furthermost downstream water column compartment (compart-
ment five). The inability for the six compartment model
to adequately predict the target (field) concentrations
in compartment five was due to the length of the compart-
ment (6.7 miles), and the fact that the model assumes

complete mixing and creates instantaneous equilibrium within each compartment. As a result, a ten compartment configuration was utilized to obtain the final calibration. This configuration was obtained by dividing compartments five (water column) and six (adjacent benthic) into three equal compartments. This division was performed to achieve a greater compartment sensitivity to obtain the target (field measured) concentrations.

This final configuration (based upon the data provided) accurately predicted total, dissolved and particulate concentrations for all water column and benthic compartments. The major parameters adjusted to obtain this final calibration were the percent groundwater routed through the benthic compartments, the percent advected flow from benthic to water column compartments, and the "activity" $K_d$'s were kept at field determined values. However, the calibration of this model is only the initial phase of accurately modeling this river reach, and model validation to another data set is required.

The validation process could also include a reduction of the following model limitations that were discovered during the calibration process; the need for additional organic complexes within the thermodynamic data base, the ability for the model to simulate more than one priority pollutant metal simultaneously, and the

END
FILMED

DTIC
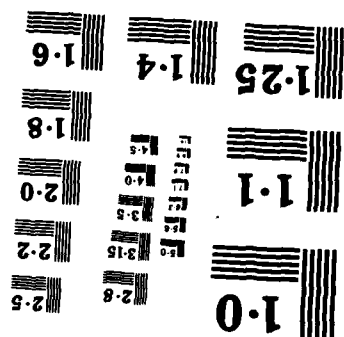
ability for the user to adjust the concentration to be obtained during the system self-purification (persistence calculation). The validation of this model could result in possible future applications and provide additional assistance to the Department of Environmental Protection, State of Connecticut in determining waste discharge allocations for present and future dischargers within this reach of the Naugatuck River.

In conclusion, the results of the study suggest that MEXAMS is a potentially powerful management tool that could be utilized for a variety of environmental problems. Future activity using the model should continue the application to actual field situations so that continued refinement of the model and appropriate modifications are made to promote its use.

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APPENDICES

APPENDIX A

DESCRIPTION OF THE MINTEQ INPUT FILE
(Felmy et al., 1983)

This appendix describes how to setup the sample description file for running the VAX and PDP 11/70 versions of MINTEQ. A detailed description of the options available to the user accompanies the file descriptions.

The file is broken into three sections. Each section is separated by a blank line. There should be three and only three blank lines in the sample file. The three sections will be called Basic Input Data, Type Modifications and Insertion of Species. The format field designations for each line are given in parenthesis following the line designation.

Section 1 - Basic Input Data

Line 1 (A80). Alphanumeric description of the sample.

Line 2 (A80). Alphanumeric description of the sample.

Line 3. Water temperature, analytical units and fixed ionic strength designation

The water temperature in degrees Celcius is entered followed by the analytical units. In the VAX free-format version, the temperature and units must be separated by a space and the units enclosed in quote marks. The PDP 11/70 version follows the designated format fields. The analytical unit designations can be either 'PPM', 'MG/1',

'MOL', or 'MEQ/L'. These designations stand for parts per million, milligrams per liter, molality and milli-equivalents per liter, respectively. The fixed ionic strength is entered following the analytical units. In the VAX version there must be a space between the analytical units and the ionic strength. If the ionic strength is not fixed, enter 0.0 following the analytical units.

Line 4[8(I1,IX)]. This line contains the run specific user options.

Option 1. The inorganic carbon input option.

   (0) = Total inorganic carbon.

   (1) = Total alkalinity.

Option 2. The Debug print option. This is generally used only when modifications have been made to the code and the values of certain arrays must be checked.

   (0) = No Debug printout.

   (1) = Prints the value of the IDX, C, IDY, GAMMA, C and Y arrays.

   (3) = Prints the NNN, NN(1), NN(2) and the IDY, GK, GK1 arrays in subroutine KCORR.

   (4) = Prints the IDX, C, IDY, L and GK arrays every iteration in subroutine SOLID and the saturation index for the solid

added to the phase assemblage in sub-
routine SOLIDX.

Option 3. The charge balance option.

    (0) = Terminates execution of the program if the
initial charge in balance is greater than
30 percent.

    (1) = Does not terminate execution regardless
of the initial computed charge imbalance.

Option 4. Considered solids and print option.

    (0) = Do not allow all of the solids in the
data base to precipitate or dissolve. The
only solids considered will be those
entered in the next input section under
type changes. Print the problem results
after the initial aqueous speciation plus
solids problem is solved and after all
Type V solids are either in equilibrium or
undersaturated.

    (1) = Allow all solids in the data base to
precipitate if they become oversaturated.
That is, designate all solids in the data
base as Type V. Print the problem results
only after the entire problem has been
solved.

    (2) = Consider all solids in the data base.

Print the problem results after the initial user specified problem has been solved and again after all Type V solids are undersaturated or in equilibrium.

(3) = Consider all solids in the data base. Print the problem results following the selection of every solid and after all of the solids are in equilibrium or undersaturated.

Option 5. The total number of iterations option.

(0) = Allow 40 iterations.

(1) = Allow 10 iterations.

(2) = Allow 100 iterations.

(3) = Allow 200 iterations.

The 100 or 200 iteration options should be selected if a large number of solids have been designated as considered solids. The ten iteration option is only useful when debugging the program.

Option 6. The pH variation option.

(0) = Do not allow the pH to automatically vary during precipitation/dissolution of solid phases.

(1) = Allow the pH to vary during precipitation/dissolution of solid phases. Not for this option to work all solid phases must

be declared Type V in the initial input.

Option 7. The fixed ionic strength option.

  (0) = Allow MINTEQ to compute the ionic
strength.

  (1) = Fix the ionic strength at the value
    designated on line 3.

Option 8. The numerical method option.

  (0) = Use only Newton-Raphson iteration.

  (1) = Use a combination of Newton-Raphson
    and a modified line search.  This
    option should only be used after
    consulting the technical manual.

Option 9.  Output Option (available only on VAX)

  (0) = Do not print on initial listing of the
    thermodynamic data.

  (1) = Print a listing of the thermodynamic data.

Line 5 [I1,1X,4(F6.2,1X)]. This line is for
input of adsorption parameters other than the mass total
and activity guesses. The first parameter on this line is
the adsorption model being used (I1 field). The options
are:

    0 - No Adsorption

    1 - Activity Kd, Langmiur isotherm
      Freundlich isotherm

2 - Constant Capacitance Double Layer Model

3 - Triple Layer Site Binding Model.

The next four inputs on this line are:

- Solid Concentration (g/l)

- Specific Surface Area (m2/g)

- Inner Layer Capacitance (F/m2)

- Outer Layer Capacitance (F/m2)

input in this order. None of the last four inputs are required for the activity Kd. The constant capacitance model does not require an outer layer capacitance. The triple layer model requires all four data inputs.

Line 6+ (17,IX,E9.3,IX,F6.2). Component input lines. There are as many of these lines as there are components. A blank line must follow the last component.

The first specification (17) is the component ID number. Component ID numbers are given in Table 3. The second specification (E9.3 field) is the total analytical mass in the units designated on line 3. The only exception occurs when the constant capacitance of triple layer models are used. In such cases the analytical mass for the surface sites (SOH1 or SOH2 components) must be specified in sites per gram. The third specification on this line is a guess at the log of the component activity. If you leave this field blank the initial estimate of the activity will be the analytical molality divided by 100. Remember you need one line for every

component and a blank line after the last component.

## Section 2 - Type Modification

This section is for changing the default species designations. The default type specification have been described in Section 5.

The first line of this section contains the first species type designation and the number of species of this type Format (I3, 1X, I3). The type designations can range from two to six. Then for each species of the entered type, a line is included (I7, 1X, E9.3, 1X, F6.2) designating information for that species. The first field specification is for the species ID number. Species ID numbers for components (Type I) are given in Table 3. All other species ID numbers can be found in the listing of Thermodynamic Data given in the MINTEQ Technical Report. The next two specifications are for the new log K and enthalpy of reaction. These are both optional and if not included the default values in the thermodynamic data base are used. A blank line also ends this section. In the case of Type IV species with an initial mass total (in moles/l) there is an additional input field for the initial mass. This input field follows the input of the enthalpy of reaction resulting in four inputs on one line. The input format for Type IV species is (I7, 1X, E9.3, 1X. F6.2, 1X, E10.3). For examples of necessary species modifications to solve specific problems see

Section 5.

## Section 3 - Insertion of Species Not in the Data Base

The first line is for designating the species type
and the number of new species of this type (Format I3,
1X, I3). The species type can only range from two to six.
The next lines contain the data for the new species of
the specified type. There are three lines for each
species. The first line of species data is in Format (I7,
1X, A12, 2F10.4, 2F8.3, 3F5.2, F9.4). The format fields
correspond to the following data: ID number, name, en-
thalpy of reaction, log K, minimum log K, maximum log K,
charge, Debye-Huckel A parameter, Debye-Huckel B
parameter and molecular weight respectively. Only the ID
number and log K are absolutely essential. For a descrip-
tion of the Debye-Huckel parameters see the MINTEQ Tech-
nical Report. The second line of data is in Format [F5.2,
1X, I1, 1X, 6(F7.3, 1X, I3, 1X)]. The format fields
correspond to: carbonate alkalinity factor, number of
components in the reaction and the stoichiometry and ID
number for up to six components. The carbonate alkalinity
factor is only useful if the input inorganic carbon is an
alkalinity value. A description of the carbonate
alkalinity factor is given in the MINTEQ Technical
Report. The third line is in Format [3(F7.3, 1X, I3, 1X)]
and is merely a continuation of the component entries for
the inserted species. In the VAX version, the third line

is in format [3(F7.3, 1X, I3, 1X), I1, 3(F7.3, 1X, I3, 1X)]. The format field beginning with I1 is for inserting species information into the "B" matrix. Such information is only useful when the component stoichiometries in the mass action expressions are different from the stoichiometries in the mass balance equation. The latter format fields correspond to the number of components in the "B" matrix, stoichiometry of the component and component ID number. This section is also terminated with a blank line.

# APPENDIX B

## DESCRIPTION OF THE EXAMS INPUT FILE
### (Burns et al., 1981)

The narrative associated with each database references
the format codes listed below.

| Code | Format |
|------|--------|
| 1 | 60 characters, left justified. Format: (60A1) |
| 2 | Columns 1-5 right justified. Format: (20I5) |
| 3 | Column 1, one character/record. The maximum number of records is equal to the number of compartments. Format: (A1) |
| 4 | Columns 1-10. Format: (F10.0) |
| 5 | Each record contains 8 10-column fields, maximum 2 records per variable. Format: (8F10.0) |

|  | Columns | Compartment |
|--|---------|-------------|
| Record 1 | 1-10 | 1 |
|  | 11-20 | 2 |
|  | . | . |
|  | . | . |
|  | . | . |
| Record 2 | 1-10 | 9 |
| (if needed) | 11-20 | 10 |

| Code | Format |
|------|--------|
| 6 | Five record layout containing 39 values. Four records contain eight 10-column fields; the fifth contains seven. Format: (8F20.0) |

|  | Columns | Value |
|--|---------|-------|
| Record 1 | 1-10 | 1 |
|  | 11-20 | 2 |
|  | . | . |
|  | . | . |
|  | . | . |
|  | 71-80 | 8 |
| Record 2 | 1-10 | 9 |
|  | . | . |
|  | . | . |
|  | . | . |

|  | 71-80 | 16 |
| --- | --- | --- |
|  | . | . |
|  | . | . |
|  | . | . |
| Record 5 | 1-10 | 33 |
|  | . | . |
|  | . | . |
|  | . | . |
|  | 61-70 | 39 |

7       The number of records is equal to NSPEC1 or NSPEC2 divided by 16. Each record contains 16 five-column fields. For JFRADG and ITOADG use NSPEC1 and for JTURBG and ITURBG use NSPEC2. Each field is right justi-fied. Format: (20I5)

|  | Columns | &lt;Par&gt; |
| --- | --- | --- |
| Record 1 | 1-5 | 1 |
|  | 6-10 | 2 |
|  | . | . |
|  | . | . |
|  | . | . |
|  | 76-80 | 16 |
| Record 2 | 1-5 | 17 |
|  | . | . |
|  | . | . |
|  | . | . |
| Record n | 41-50 | 29 |
|  | 51-60 | 30' |

8       Format: (5(I1,1X))

|  | Column | Flag |
| --- | --- | --- |
|  | 1 | 1 |
|  | 3 | 2 |
|  | 5 | 3 |
|  | 7 | 4 |
|  | 9 | 5 |

9       Format: (8F10.0)

|  | Columns | Value |
| --- | --- | --- |
|  | 1-10 | 1 |
|  | 11-20 | 2 |
|  | 21-30 | 3 |

10          Format: (8F10.0)

|         | Columns | Value |
|---------|---------|-------|
|         | 1-10    | 1     |
|         | 11-20   | 2     |
|         | 21-30   | 3     |
|         | 31-40   | 4     |

11          Format: (8F10.0)

|         | Columns | Value |
|---------|---------|-------|
|         | 1-10    | 1     |
|         | 11-20   | 2     |

12          The number of records is equal to
            NSPEC1 or NSPEC2 divided by eight.
            Each record contains eight 10-column
            fields. For ADVPRG use NSPEC1 and
            for XSTURG, CHARLG, and DSPG use
            NSPEC2. Format:(8F10.0)

|          | Columns | Value |
|----------|---------|-------|
| Record 1 | 1-10    | 1     |
|          | 11-20   | 2     |
|          | .       | .     |
|          | .       | .     |
|          | .       | .     |
|          | 71-80   | 8     |
| Record 2 | .       | .     |
| .        | .       | .     |
| .        | .       | .     |
| Record n | 41-50   | 29    |
|          | 51-60   | 30    |

Creating or Changing the User Run Information


This sequential file contains chemical name, ecosystem, name, and loads.


Record 1:  (CHEM1)  Chemical name - three characters
                    maximum.  Format:(A3)

Record 2:  (ECO1)  Ecosystem name - three characters
                    maximum.  Format: (A3)

Record 3:  (NLOAD)  Number of Loads.  Format: (I5)

Record 4,...,NLOAD+3:(I, STRLDG, NPSLDG, PCPLDG, DRFLDG,
                    IFLLDG)  Each of NLOAD records
                    contain the load number and the
                    Ith STRLDG, NPSLDG, PCPLDG,
                    DRFLDG, IFLLDG. Format
                    (I5,5F10.0)

                    STRLDG - Stream loadings.
                    NPSLDG - Non-point source loadings.
                    PCPLDG - Precipitation loadings.
                    DRFLDG - Drift loadings
                    IFLLDG - Interflow loadings.


|  | Columns | Field |
|---|---|---|
| Record 4 | 1-5 | I |
|  | 6-15 | STRLDG(I) |
|  | 16-25 | NPSLDG(I) |
|  | 26-35 | PCPLDG(I) |
|  | 36-45 | DRFLDG(I) |
|  | 46-55 | IFLLDG(I) |

Creating or Changing the Environment Database

The compartment parameter data are located in the follow-
ing sequential record layout. (The format code list
provides detailed format specifications.)

Record: (SYSTYP) Ecosystem name, maximum 60 characters
Format: 1

Record: (KOUNT) Number of compartments, maximum number
of compartments is NPX, which is
fixed for a particular installation.
Format: 2

Record: (TYPEE) The next KOUNT records each contain a
one character compartment code,
KOUNT the number of compartments.
Format: 3

Record: (LATG) Ecosystem latitude, columns 1-10,
degrees and seconds as whole number
and decimal fraction, e.g. 10.15.
Format: 4

Record: (WINDG) Wind velocity per compartment, eight
per record. Format: 5

Record: (VOLG) Total environmental volume per compart-
ment. Format: 5

Record: (AREAG) Area of each ecosystem compartment.
Format: 5

Record: (DEPTHG) Average depth of each compartment.
Format: 5

Record: (STDLOG) Stream flow entering ecosystem compart-
ments. Format: 5

Record: (STSEDG) Stream-born sediment load entering
ecosystem compartments. Format: 5

Record: (NPSFLG) Non-point-source water flow entering
ecosystem compartments. Format: 5

Record: (NPSEDG) Non-point-source sediment loads enter-
ing ecosystem compartments. Format: 5

Record: (INTFLG) Interflow (groundwater seepage) enter-
ing each ecosystem compartment.

Format: 5

Record: (RAING)  Average rainfall in geographic area of
system. Columns 1-10. Format: 4

Record: (CLOUDG)  Average cloudiness in tenths of full
sky cover.  Columns 1-10. Format: 4

Record: (WLAMG)  Temporally averaged spectral irradiance
immediately below the water surface.
This is five record layout containing
39 values, ten columns per value,
eight values per record. Format: 6

Record: (DFACG)  Distribution function (optical path)
for each compartment. Format: 5

Record: (EVAPG)  Evaporative water losses from ecosystem
compartments. Format: 5

Record: (SDCHRG)  For water column compartments the
suspended sediment concentration; for
benthic sediment compartments the bulk
density of the bottom sediment.
Format: 5

Record: (PCTWAG)  Percent water in bottom sediments of
benthic compartments. Elements corres-
ponding to water column compartments
are not used (dummy values). Format: 5

Record: (NSPEC1)  Number of active advective transport
pathways. Format: 2

Record: (JFRADG)  Source compartment (J) for advective
flow. Format: 7

Record: (ITOADG)  Receiving compartment (I) for advective
flow. Format: 7

Record: (ADVPRG)  Proportion of total advective flow from
compartment J that flows to compart-
ment I. Format: 12

Record: (NSPEC2)  Number of active dispersive transport
pathways. Format: 2

Record: (JTURBG)  Source compartment for dispersive flow.
Format: 7

Record: (ITURBG)  Receiving compartment for dispersive
flow. Format: 7

Record: (XSTURG)  Cross-sectional areas for dispersive
exchanges. Format: 12

Record: (CHARLG)  Characteristic length of dispersive
exchange pairings. Format: 12

Record: (DSPG)  Eddy dispersion coefficients for
dispersive exchange pairings.
Format 12

Record: (FROCG)  Organic carbon content of compartment
sediments. Format: 5

Record: (CECG)  Cation exchange capacity of sediments
in each compartment. Format: 5

Record: (AECG)  Anion exchange capacity of sediments in
each compartment. Format: 5

Record: (TCELG)  Average temperature of ecosystem
compartments. Format: 5

Record: (PHG)  Negative value of log of temporal
average of [H+] concentration for each
compartment. Format: 5

Record: (POHG)  Negative value of log of temporally
averaged [OH-] concentration for each
compartment. Format: 5

Record: (OXRADG)  Molar concentration of environmental
oxidants in each ecosystem compart-
ment Format: 5

Record: (BIOMSG)  Total actively sorbing biomass in each
compartment. Format: 5

Record: (PLRAG)  Planktonic fraction of total biomass in
each compartment. Format: 5

Record: (BIOTMG)  Biotemperature in each compartment.
Format: 5

Record: (BACTOG)  Bacterial population density in each
compartment. Format: 5

Record: (ACBAXG)  Proportion of bacterial population that
actively degrades toxicant. Format: 5

Record: (KO2G)  Rearation parameter in each compart-
ment. Format: 5

Record: (CMPETG)  Single-valued zenith light extinction
                  coefficient for water columns, dummy
                  variable for benthic compartments.
                  Format: 5

Record: (DOCG)    Dissolved organic carbon concentration
                  in water column compartments, dummy
                  variable in benthic compartments.
                  Format: 5

Record: (CHLG)    Concentration of chlorophyll and
                  chlorophyll-like pigments in water
                  column compartments, dummy variable
                  in benthic compartments. Format: 5

APPENDIX C


MINTEQ Output

MINTEQ=MINTEQ=MINTEQ=MINTEQ MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINTEQ=MINT
EQ=MINTEQ=

ONAUGATUCK RIVER CONDITIONS (16-17 AUGUST 1983) COMPARTMENT 1  ZN-CU-PB ADSORPTION
KD MODEL  MATRIX OBTAINED FROM BEST AVAILABLE DATA PH=7.14
T = 25.00 MG/L

```
0 0 1 0 0 0 0 0       0
CHARGE BALANCE: UNSPECIATED
    SUM OF CATIONS= 2.203E-03  SUM OF ANIONS = 2.863E-03
    PERCENT DIFFERENCE =  -13.04   (CATIONS - ANIONS)/(ANIONS + CATIONS)
ITERATIONS DURING SOLVE
```

| ITER | NAME | TOTAL MOL | DIFF FXN | LOG ACTVTY |
|------|------|-----------|----------|------------|
| 1 | CA | 4.991E-04 | -2.910E-04 | -3.80000 |
| 2 | CA | 4.991E-04 | -6.766E-05 | -3.38469 |
| 3 | CA | 4.991E-04 | 1.439E-04 | -3.32420 |
| 4 | CA | 4.991E-04 | 2.858E-04 | -3.43010 |
| 5 | CA | 4.991E-04 | -1.933E-04 | -3.62025 |
| 6 | CA | 4.991E-04 | 3.429E-06 | -3.41555 |

OUTPUT DATA: ITERATIONS = 6

| ID | NAME | ANAL MOL | CALC MOL | ACTIVITY | LOG ACTVTY | GAMMA | NEW LOGK | DIFF FXN |
|----|------|----------|----------|----------|------------|-------|----------|----------|
| 150 | CA | 4.991E-04 | 4.815E-04 | 3.817E-04 | -3.41830 | .792686 | .1009 | -3.620E-07 |
| 460 | MG | 1.440E-04 | 1.393E-04 | 1.107E-04 | -3.95593 | .794378 | .1000 | -1.034E-07 |
| 500 | NA | 8.222E-04 | 8.211E-04 | 7.734E-04 | -3.11159 | .941939 | .0260 | -9.644E-07 |
| 140 | CO3 | 5.703E-04 | 3.792E-07 | 2.996E-07 | -6.52348 | .789951 | .1024 | -9.605E-08 |
| 732 | SO4 | 2.603E-04 | 2.408E-04 | 1.891E-04 | -3.72333 | .785348 | .1049 | -1.954E-07 |
| 180 | CL | 1.072E-03 | 1.072E-03 | 1.008E-03 | -2.99650 | .940572 | .0266 | -2.252E-07 |
| 90 | H3BO3 | 1.352E-06 | 3.341E-06 | 1.342E-06 | -5.87224 | .000697 | .0003 | 4.353E-12 |
| 410 | K | 7.904E-05 | 7.892E-05 | 7.423E-05 | -4.12945 | .940572 | .0266 | -1.660E-08 |
| 580 | PO4 | 5.167E-06 | 1.940E-11 | 1.137E-11 | -10.94412 | .586236 | .2319 | -2.220E-09 |
| 770 | H4SiO4 | 8.658E-05 | 8.643E-05 | 6.449E-05 | -4.06305 | .000697 | .0003 | 4.065E-10 |
| 231 | CU+2 | 2.578E-07 | 1.223E-07 | 9.686E-08 | -7.01385 | .791776 | .1014 | -9.856E-11 |
| 950 | ZN | 2.677E-07 | 1.671E-07 | 1.323E-07 | -6.87842 | .940473 | .0267 | -1.273E-10 |
| 492 | NO3 | 1.143E-04 | 1.142E-04 | 1.074E-04 | -3.96888 | .940473 | .1014 | -2.409E-08 |
| 470 | MN+2 | 6.463E-07 | 6.220E-07 | 4.925E-07 | -6.30758 | .791776 | .1014 | -4.708E-10 |
| 281 | FE+3 | 2.932E-06 | 2.455E-14 | 1.545E-15 | -14.12233 | .606033 | .2175 | -6.464E-10 |
| 600 | PB | 2.896E-08 | 2.866E-09 | 1.010E-09 | -8.99549 | .785813 | .1047 | -1.150E-12 |
| 2 | H2O | 0 | -9.247E-06 | 9.999E-01 | -.00003 | 1.000000 | .0000 | 0 |
| 991 | SOH2 | 0 | -1.791E-07 | 0.000E+00 | 0 | 1.000000 | 0 | 0 |
| 990 | SOH1 | 0 | -7.613E-08 | 0.000E+00 | 0 | 1.000000 | 0 | 0 |
| 330 | H | 0 | -6.425E-04 | 7.244E-08 | -7.14000 | .945873 | 7.1400 | 0 |

SPECIES  TYPE 1 - COMPONENTS

| ID | NAME | CALC MOL | ACTIVITY | LOG ACTVTY | GAMMA | NEW LOGK | DM |
|----|------|----------|----------|------------|-------|----------|-----|
| 150 | CA | 4.815E-04 | 3.817E-04 | -3.41830 | .792686 | .101 | 0 |
| 460 | MG | 1.393E-04 | 1.107E-04 | -3.95593 | .794378 | .100 | 0 |
| 500 | NA | 8.211E-04 | 7.734E-04 | -3.11159 | .941939 | .026 | 0 |
| 140 | CO3 | 3.792E-07 | 2.996E-07 | -6.52348 | .789951 | .102 | 0 |
| 732 | SO4 | 2.408E-04 | 1.891E-04 | -3.72333 | .785348 | .105 | 0 |
| 180 | CL | 1.072E-03 | 1.008E-03 | -2.99650 | .940572 | .027 | 0 |
| 90 | H3BO3 | 3.341E-06 | 1.342E-06 | -5.87224 | .000697 | .000 | 0 |
| 410 | K | 7.892E-05 | 7.423E-05 | -4.12945 | .940572 | .027 | 0 |
| 580 | PO4 | 1.940E-11 | 1.137E-11 | -10.94412 | .586236 | .232 | 0 |
| 770 | H4SiO4 | 8.643E-05 | 6.449E-05 | -4.06305 | .000697 | .000 | 0 |
| 231 | CU+2 | 1.223E-07 | 9.686E-08 | -7.01385 | .791776 | .101 | 0 |
| 950 | ZN | 1.671E-07 | 1.323E-07 | -6.87842 | .791776 | .101 | 0 |
| 492 | NO3 | 1.142E-04 | 1.074E-04 | -3.96888 | .940473 | .101 | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9912310 | SOH-CU | 1.535E-07 | 1.535E-07 | -8.81385 | 1.000000 | .200 | 0 |
| 3307320 | HSO4 - | 1.412E-09 | 1.330E-09 | -8.87626 | .941922 | 2.013 | 4.910 |
| 3303800 | HPO4 -2 | 2.317E-06 | 1.828E-06 | -5.73812 | .788717 | 12.449 | -3.530 |
| 3303801 | H2PO4 - | 2.262E-06 | 2.132E-06 | -5.67112 | .942758 | 19.579 | -4.520 |
| 33000020 | OH- | 1.474E-07 | 1.387E-07 | -6.85803 | .940964 | -13.972 | 13.345 |
| 3307700 | H3SIO4 - | 1.494E-07 | 1.407E-07 | -6.85183 | .941447 | -9.903 | 8.935 |
| 3307701 | H2SIO4 -2 | 5.044E-12 | 3.984E-12 | -11.39966 | .789951 | -21.514 | 29.714 |
| 3309900 | H2BO3 - | 1.132E-08 | 1.064E-08 | -7.97305 | .939974 | -9.214 | 15.935 |
| 4603300 | MGOH + | 2.661E-09 | 2.511E-09 | -8.60007 | .943747 | -11.759 | 3.224 |
| 4601400 | MGCO3 AQ | 3.162E-08 | 3.165E-08 | -7.49968 | 1.000697 | 2.979 | -2.022 |
| 4601401 | MGHCO3 + | 6.337E-07 | 5.966E-07 | -6.22429 | .941447 | 11.421 | -2.430 |
| 4607320 | MGSO4 AQ | 6.719E-06 | 6.722E-06 | -5.42926 | 1.000697 | 2.250 | -1.399 |
| 4605800 | MGPO4 - | 5.183E-09 | 4.806E-09 | -8.31105 | .942758 | 6.615 | 3.100 |
| 4605801 | MGH2PO4 + | 8.157E-09 | 7.690E-09 | -8.11405 | .942758 | 21.092 | -1.120 |
| 4605802 | MGHPO4 AQ | 3.512E-07 | 3.512E-07 | -6.82005 | 1.000697 | 15.220 | -.230 |
| 1503300 | CAOH + | 1.409E-09 | 1.329E-09 | -8.87633 | .943302 | -12.573 | 14.535 |
| 1501400 | CAHCO3 + | 1.944E-06 | 1.834E-06 | -5.73669 | .943302 | 11.370 | -1.790 |
| 1501401 | CACO3 AQ | 1.624E-07 | 1.625E-07 | -6.78917 | 1.000697 | 3.152 | 4.030 |
| 1507320 | CASO4 AQ | 4.469E-05 | 4.470E-05 | -4.83263 | 1.000697 | 2.309 | -1.470 |
| 1505800 | CAHPO4 AQ | 3.822E-07 | 3.825E-07 | -6.41742 | 1.000697 | 15.085 | -.230 |
| 1505801 | CAPO4 - | 1.325E-08 | 1.249E-08 | -7.90342 | .942758 | 6.485 | -3.100 |
| 1505802 | CAH2PO4 + | 2.204E-08 | 2.078E-08 | -7.68242 | .942758 | 20.986 | -.120 |
| 5001400 | NACO3 - | 4.555E-09 | 4.295E-09 | -8.36707 | .942758 | -1.294 | 0.911 |
| 5001401 | NAHCO3 AQ | 2.017E-07 | 2.010E-07 | -6.69507 | 1.000697 | 10.080 | 0 |
| 5007320 | NASO4 - | 7.775E-07 | 7.330E-07 | -6.13492 | .942758 | .726 | 1.120 |
| 5005800 | NAHPO4 - | 4.923E-09 | 2.756E-09 | -8.55971 | .942758 | 12.662 | 0 |
| 5005801 | NAH2PO4 + | 1.046E-07 | 9.864E-08 | -7.00596 | .942758 | .872 | 2.250 |
| 4107320 | KSO4 - | 2.032E-10 | 2.870E-10 | -9.57357 | .942758 | 12.666 | 0 |
| 4105800 | KHPO4 - | 3.526E-10 | 7.724E-10 | -9.17236 | .788717 | -2.087 | 10.398 |
| 2813100 | FEOH +2 | 3.973E-15 | 3.748E-15 | -14.42645 | .942758 | 17.806 | -7.300 |
| 2815800 | FEHPO4 + | 1.295E-14 | 1.187E-14 | -15.63863 | .942389 | 3.946 | 3.910 |
| 2817320 | FESO4 + | 2.912E-16 | 2.297E-16 | -17.98533 | .788717 | -1.563 | 5.600 |
| 2811800 | FECL +2 | 1.098E-16 | 1.034E-22 | -21.98183 | .942309 | 2.156 | 0 |
| 2811801 | FECL2 + | 1.042E-22 | 1.043E-22 | -5.51239 | .942758 | -1.130 | 0 |
| 2813301 | FECL3 AQ | 3.260E-06 | 3.075E-06 | -6.30241 | .942758 | -13.600 | 0 |
| 2813302 | FEOH2 + | 4.981E-07 | 4.984E-07 | -7.16244 | .942758 | -21.574 | 0 |
| 2813303 | FEOH3 AQ | 7.297E-08 | 6.880E-08 | -14.36645 | .789951 | 25.082 | 0 |
| 2815801 | FEH2PO4 +2 | 4.444E-15 | 1.301E-15 | -16.14899 | .941520 | 5.446 | 4.600 |
| 2817321 | FE(SO4)2 - | 7.537E-17 | 7.096E-17 | -16.91472 | .381308 | -2.531 | 13.500 |
| 2013304 | FE2(OH)2+4 | 3.192E-17 | 2.217E-17 | -20.10710 | .221669 | -5.646 | 14.300 |
| 2813305 | FE3(OH)4+5 | 3.525E-20 | 7.814E-21 | -8.69708 | .942389 | .041 | 0 |
| 4701800 | MNCL + | 2.132E-09 | 2.009E-09 | -12.25958 | 1.000697 | .279 | 0 |
| 4701801 | MNCL2 AQ | 5.497E-13 | 5.501E-13 | -15.60208 | .942389 | -10.564 | 14.399 |
| 4701802 | MNCL3 - | 1.034E-10 | 2.506E-16 | -19.68766 | .942389 | -34.774 | 1.396 |
| 4703300 | MNOH + | 1.178E-20 | 1.747E-10 | -7.77090 | 1.000697 | 2.260 | 2.170 |
| 4703301 | MN(OH)3 -1 | 6.694E-08 | 1.695E-08 | -13.64534 | 1.000697 | .600 | -.396 |
| 4707320 | MNSO4 AQ | 2.261E-14 | 2.263E-14 | -8.37105 | .942389 | 11.626 | 0 |
| 4704920 | MN(NO3)2AQ | 4.516E-09 | 4.255E-09 | -6.80733 | .942389 | 6.730 | 0 |
| 4701400 | MNHCO3 + | 1.557E-07 | 1.558E-07 | -10.23081 | .785813 | 9.915 | 0 |
| 2311400 | CUCO3 AQ | 7.479E-11 | 5.877E-11 | -9.58005 | .941447 | .456 | 6.650 |
| 2311401 | CUCO3)2-2 | 2.792E-10 | 2.626E-10 | -12.84686 | .000697 | .160 | 10.560 |
| 2311801 | CUCL + | 1.422E-13 | 1.423E-13 | -18.29336 | .941447 | -2.264 | 13.690 |
| 2311802 | CUCL2 AQ | 5.406E-19 | 5.089E-19 | -23.58986 | .788717 | -4.487 | 17.780 |
| 2311003 | CUCL3 - | 3.360E-24 | 5.571E-24 | -7.87308 | .941117 | -7.971 | 0 |
| 2313300 | CUCL4 -2 | 1.205E-03 | | | | | |

| SPECIES ID | NAME | TYPE | CALC MOL | LOG MOL | NEW LOGK | | | |
|---|---|---|---|---|---|---|---|---|
| 9501800 | ZNCL + | | 3.813E-10 | 3.590E-10 | -9.44492 | 941447 | .456 | 7.790 |
| 9501801 | ZNCL2 AQ | | 3.787E-13 | 3.789E-13 | -12.42142 | 1.000697 | .450 | 8.500 |
| 9501802 | ZNCL3 - | | 4.553E-16 | 4.286E-16 | -15.36792 | 941447 | .526 | 9.560 |
| 9501803 | ZNCL4 -2 | | 2.739E-19 | 2.161E-19 | -10.65542 | 788717 | .302 | 10.960 |
| 9503300 | ZNOH + | | 2.127E-09 | 2.002E-09 | -8.69845 | 941520 | .934 | 13.399 |
| 9503301 | ZN(OH)2 AQ | | 3.179E-10 | 3.181E-10 | 49.747 | 000697 | -8.899 | 0 |
| 9503302 | ZN(OH)3 - | | 1.475E-14 | 1.388E-14 | -13.85750 | 941520 | -28.373 | 0 |
| 9503303 | ZN(OH)4 -2 | | 3.865E-20 | 3.037E-20 | -19.51753 | 941520 | -41.094 | 0 |
| 9501804 | ZNOHCL AQ | | 6.092E-11 | 6.096E-11 | -10.21495 | 785813 | -7.480 | 0 |
| 9507320 | ZNSO4 AQ | | 5.861E-09 | 5.865E-09 | -8.23175 | 1.000697 | -7.460 | 1.360 |
| 9507321 | ZN(SO4)2 -2 | | 1.147E-11 | 1.014E-11 | -11.04507 | 785813 | 2.370 | 0 |
| 9501400 | ZNCO3 + | | 7.661E-09 | 7.213E-09 | -8.14190 | 941520 | 12.426 | 0 |
| 9501401 | ZNCO3 AQ | | 7.903E-09 | 7.909E-09 | -8.10190 | 000697 | 5.300 | 0 |
| 9501402 | ZN(CO3)2 -2 | | 4.446E-11 | 4.055E-11 | -10.29538 | 785813 | 9.735 | 0 |
| 6001800 | PBCL + | | 4.307E-11 | 4.076E-11 | -10.39199 | 941520 | 1.626 | 4.380 |
| 6001801 | PBCL2 AQ | | 6.475E-14 | 6.479E-14 | -13.18849 | 1.000697 | .800 | 1.080 |
| 6001802 | PBCL3 - | | 5.498E-17 | 5.176E-17 | -16.28599 | 785813 | .725 | 2.170 |
| 6001803 | PBCL4 -2 | | 3.186E-20 | 2.503E-20 | -19.60119 | 785813 | 1.485 | 3.530 |
| 6073300 | PBOH + | | 2.286E-10 | 2.719E-10 | -9.56552 | 941520 | 10.745 | 0 |
| 6003301 | PB(OH)2 AQ | | 1.159E-12 | 1.460E-12 | -11.83554 | 1.000697 | -7.684 | 0 |
| 6003302 | PB(OH)3 - | | 2.458E-16 | 2.314E-16 | -15.63557 | 941520 | -17.120 | 0 |
| 6003303 | PB2OH+3 | | 1.058E-17 | 1.152E-18 | -17.21101 | 581390 | -28.034 | 0 |
| 6004920 | PBNO3 + | | 1.705E-12 | 1.606E-12 | -11.79437 | 941520 | -6.124 | 0 |
| 6007320 | PBSO4 AQ | | 1.074E-10 | 1.074E-10 | -9.96882 | 1.000697 | -1.196 | 0 |
| 6003304 | PB3(OH)4+2 | | 6.282E-23 | 4.937E-23 | -22.30658 | 785813 | 2.750 | 28.500 |
| 6001401 | PBCO3 AQ | | 5.257E-09 | 5.261E-09 | -8.27897 | 1.000697 | -23.775 | 0 |
| 6003305 | PB(OH)4 -2 | | 1.334E-21 | 1.335E-21 | -20.13460 | 785813 | 7.240 | 0 |
| 6007321 | PB(SO4)2 -2 | | 3.357E-13 | 1.066E-13 | -12.97214 | 785813 | -39.594 | 0 |
| 6001402 | PBHCO3 + | | 3.691E-10 | 3.476E-10 | -9.45897 | 941520 | 3.575 | 0 |
| 3301400 | HCO3 - | | 4.917E-04 | 4.675E-04 | -3.33392 | 942758 | 13.226 | 0 |
| 3301401 | H2CO3 AQ | | 7.500E-05 | 7.505E-05 | -4.12466 | 000697 | 10.355 | -3.617 |
| 9903500 | SOH-ZN | | 7.613E-08 | 7.613E-08 | -7.11842 | 1.000000 | 16.679 | -2.247 |
| 9916000 | SOH-PB | | 2.160E-08 | 2.160E-08 | -7.66549 | 1.000000 | 1.330 | 0 |

| | | | TYPE III - FIXED SOLIDS | | | | |
|---|---|---|---|---|---|---|---|
| SPECIES | TYPE | | CALC MOL | LOG MOL | NEW LOGK | | |
| ID | NAME | | | | | | |
| 2 | H2O | | -9.247E-06 | -5.034 | .000 | OH | 0 |
| 991 | SOH2 | | -1.751E-07 | -6.757 | 0 | | 0 |
| 990 | SOH1 | | -7.613E-08 | -7.118 | 0 | | 0 |
| 330 | H | | -6.425E-04 | -3.192 | 7.140 | | 0 |

| | | | TYPE VI - SPECIES NOT CONSIDERED | | | |
|---|---|---|---|---|---|---|
| SPECIES | TYPE | | CALC MOL | LOG MOL | NEW LOGK | |
| ID | NAME | | | | | |
| 3301403 | CO2(GAS) | | 2.273E-03 | -2.643 | 13.160 | OH | -.530 |

PERCENTAGE DISTRIBUTION OF COMPONENTS

| | | | | | | CA | |
|---|---|---|---|---|---|---|---|
| OCA | 96.5 | PERCENT BOUND IN SPECIES | 150 | | | CASO4 AQ | |
| | 2.9 | PERCENT BOUND IN SPECIES | 1507320 | | | | |

| | | | | | | MG | |
|---|---|---|---|---|---|---|---|
| OMG | 96.8 | PERCENT BOUND IN SPECIES | 460 | | | MGSO4 AQ | |
| | 2.6 | PERCENT BOUND IN SPECIES | 4607320 | | | | |

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OSO4
        92.6   PERCENT BOUND IN SPECIES  4607320   SO4
         1.4   PERCENT BOUND IN SPECIES            MGSO4 AQ
         5.6   PERCENT BOUND IN SPECIES  1507320   CASO4 AQ

OCL
       100.0   PERCENT BOUND IN SPECIES      180   CL

OH3BO3
        99.2   PERCENT BOUND IN SPECIES       90   H3BO3

OK
        99.9   PERCENT BOUND IN SPECIES      410   K

OPO4
        44.9   PERCENT BOUND IN SPECIES  3305800   HPO4 -2
        43.8   PERCENT BOUND IN SPECIES  3305801   H2PO4 -
         2.9   PERCENT BOUND IN SPECIES  4605802   IMHPO4 AQ
         7.4   PERCENT BOUND IN SPECIES  1505800   CAHPO4 AQ

OH4SIO4
        99.8   PERCENT BOUND IN SPECIES      770   H4SIO4

OCU+2
        14.3   PERCENT BOUND IN SPECIES      231   CU+2
        17.9   PERCENT BOUND IN SPECIES  9912310   SOH-CU
        18.2   PERCENT BOUND IN SPECIES  2311400   CUCO3 AQ
         1.7   PERCENT BOUND IN SPECIES  2313300   CUOH +
        44.9   PERCENT BOUND IN SPECIES  2313301   CUIOH12 AQ
         2.6   PERCENT BOUND IN SPECIES  2311402   CUICO3 +

OZN
        62.4   PERCENT BOUND IN SPECIES      950   ZN
         2.2   PERCENT BOUND IN SPECIES  9507320   ZNSO4 AQ
         2.9   PERCENT BOUND IN SPECIES  9501400   ZNHCO3 +
         3.0   PERCENT BOUND IN SPECIES  9501401   ZNCO3 AQ
        28.4   PERCENT BOUND IN SPECIES  9909500   SOH-ZN

ONO3
       100.0   PERCENT BOUND IN SPECIES      492   NO3

OMN+2
        96.3   PERCENT BOUND IN SPECIES      470   MN+2
         2.6   PERCENT BOUND IN SPECIES  4707320   MNSO4 AQ

OFE+3
        85.1   PERCENT BOUND IN SPECIES  2813301   FEOH2 +
        13.0   PERCENT BOUND IN SPECIES  2813302   FEOH3 AQ
         1.9   PERCENT BOUND IN SPECIES  2813303   FEOH4 -

OPB
         4.4   PERCENT BOUND IN SPECIES      600   PB
        18.2   PERCENT BOUND IN SPECIES  6001401   PBHCO3 AQ
         1.3   PERCENT BOUND IN SPECIES  6001402   PBHCO3 +
        74.0   PERCENT BOUND IN SPECIES  6010000   SOH-PB
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0
0SOH2
                        87  7      PERCENT BOUND IN SPECIES 9912310    SOH-CU
                        12  3      PERCENT BOUND IN SPECIES 9916000    SOH-PB
0
0SOH1
                       100  0      PERCENT BOUND IN SPECIES 9909500    SOH-ZN
0
OH
                        76  5      PERCENT BOUND IN SPECIES 3301400    HCO3 -
                        23  3      PERCENT BOUND IN SPECIES 3301401    H2CO3 AQ
0  IDX   NAME           AQUEOUS MASS   SORBED MASS      PRECIPITATED MASS
   150   CA             4.987E-04      0                0
   460   MG             1.139E-04      0                0
   500   NA             8.221E-04      0                0
   140   CO3            5.702E-04      0                0
   732   SO4            2.601E-04      0                0
   180   CL             1.072E-03      0                0
    90   H3BO3          1.152E-06      0                0
   410   K              7.902E-05      0                0
   580   PO4            0.164E-06      0                0
   770   H4SIO4         0.653E-05      0                0
   231   CU+2           7.012E-07      1.535E-07        0
   950   ZN             1.915E-07      7.613E-08        0
   192   NO3            1.142E-04      0                0
   470   MN+2           6.456E-07      0                0
   281   FE+3           3.832E-06      0                0
   600   PB             7.360E-09      2.160E-08        0
     2   H2O            0.247E-06      0                0
   330   H              6.425E-04      0                0

CHARGE BALANCE  SPECIATED
     SUM OF CATIONS = 2.149E-03  SUM OF ANIONS = 2.160E-03
     PERCENT DIFFERENCE = -.43  (CATIONS - ANIONS)/(ANIONS + CATIONS)
NONCARBONATE ALKALINITY =       0
IONIC STRENGTH = 3.026E-03
SATURATION INDICES FOR ALL MINERALS AND SOLIDS
    ID       NAME          LOG SI   LOG K    MIN LOCK   MAX LOCK   LOG IAP    DH
  6015000  ANHYDRITE        -2.505    4.637     0          0        -7.142    3.769
  5015000  ARAGONITE        -1.606    8.336     0          0        -9.942    2.615
  5046000  ARTINITE        -9.755    -9.600     0          0         -.155   28.742
  2046000  BRUCITE         -6.168   -16.772     0          0        10.324   25.840
  5015001  CALCITE         -1.467     8.475     0          0        -9.942    2.565
  2077000  CHALCEDONY        .540     3.533     8.560      0        -4.063   -4.615
  3646000  CHRYSOTILE      -9.347   -32.108     0          0        22.046   52.485
  8246000  CLINOENSTITE    -5.077   -11.338   -10.972      0         6.261   20.015
  2077001  CRISTOBALITE     -.476    -3.587     0          0        -4.063   -5.500
  8215000  DIOPSIDE        -6.826   -19.086     0        -11.632    13.060   32.280
  5015002  DOLOMITE        -3.421    17.000     0          0       -20.421   -5.500
  6046000  EPSOMITE        -5.539     2.140     0          0         7.679   32.290
  8646003  SEPIOLITE(C)    -7.454   -15.913     0          0         8.459   -2.820
  2028100  FERRIHYDRITE     2.407    -4.891    -1.557     -4.996     7.298   27.268
  4128100  FCHH12 7CL 3     2.297     3.040     0          0         4.257    0
  6028100  FE2(SO4)3       -42.995    -3.560     650        0       -39.415   59.120
  8046000  FORSTERITE      -11.713   -28.728     0          0        16.585   48.510
  2028102  GOETHITE          4.790      .500     0          0         7.293   14.480
  6015001  GYPSUM           -2.204     4.118     0          0        -7.142   
```

| | | | | | | |
|---|---|---|---|---|---|---|
| 6028101 | JAROSITE M | -2 014 | 12 100 | 0 | 0 | -14.114 | 55.150 |
| 8450300 | MAGADIITE | -10 113 | 14 300 | 0 | 0 | -24.413 | 0 |
| 3028101 | MAGNEHITE | -2 450 | -6 386 | 0 | 0 | 14.595 | 0 |
| 50460002 | MAGNESITE | -8 833 | 8 029 | 8 279 | 7.779 | -10.479 | 6.169 |
| 60900001 | MIRABILITE | -11 436 | 1 114 | 0 | 0 | -9.947 | -18.987 |
| 3040300 | NATRON | -4 858 | 311 | 0 | 0 | -12.747 | -15.745 |
| 5046003 | MESNUEHOMITE | 057 | 5 621 | 5 133 | 4.546 | -10.479 | 5 789 |
| 2077002 | QUARTZ | 4 006 | 4 006 | 0 | 0 | -4.063 | -6 220 |
| 8646001 | SEPIOLITE(A) | -10 321 | -18.780 | 0 | 0 | 8.459 | 0 |
| 2077003 | SIO2(A,OL) | -1 045 | 3 018 | 0 | 0 | -4.063 | -4 440 |
| 2077004 | SIO2(A,PT) | 1 353 | 2 710 | 0 | 0 | -4.063 | -3 910 |
| 7028100 | STRENGITE | 1 333 | 26 400 | 29 123 | 26.235 | -25.067 | 2 030 |
| 8646002 | TALC | -8 335 | -23 055 | -18 988 | -23.088 | 14.720 | 35 005 |
| 6090002 | THENARDITE | -9 760 | 179 | 0 | 0 | -9 947 | 572 |
| 5050001 | THERMONATR | -12 872 | 125 | 0 | 0 | -12.747 | 2 802 |
| 8215001 | TREMOLITE | -15 705 | -56 146 | 0 | 0 | 40.840 | 96 615 |
| 2047003 | PYROCROITE | -7 116 | -15 048 | 0 | 0 | 7 972 | 22 590 |
| 5047000 | RHODOCHROSIT | -2 121 | 10 410 | 11 016 | -15.361 | -12.301 | 2.079 |
| 4147000 | MNKCL2. 4H2O | -15 011 | 2 710 | 0 | 9.993 | -10.001 | -17.380 |
| 6047000 | MNSO4 | -12 700 | 569 | 0 | 0 | -40.011 | -15.480 |
| 7047000 | MN3(PO4)2 | -16 944 | 23 927 | 0 | 0 | -13.407 | -2.120 |
| 4123100 | MELANOTHALLI | -3 907 | 3 730 | 0 | -4.450 | -13.537 | 12.320 |
| 5023100 | CUCO3 | -1 374 | 9 630 | 9 650 | -9.610 | 7 266 | 0 |
| 2023100 | CU(OH)2 | -3 944 | 6 640 | 0 | -9.200 | 4.396 | 15.250 |
| 4123101 | ATACAMITE | -2 317 | -7 540 | -7.240 | -7.490 | 3 423 | 18.690 |
| 5123100 | CU2(OH)3NO3 | -4 495 | -8 240 | 0 | -9.310 | 3 795 | 17.350 |
| 6023100 | ANTLERITE | -4 279 | -8 290 | 0 | -8.900 | 11.061 | 0 |
| 6023101 | BROCHANTITE | -5 729 | -15 340 | -15.150 | -15.500 | 11.061 | 38.610 |
| 6023102 | LANGITE | 354 | -16.790 | 0 | -17.400 | 7 266 | 15.240 |
| 2R023101 | TENORITE | -13 001 | -7 620 | -7 350 | -7.890 | -3 471 | 35.575 |
| 6023103 | CUDCUSO4 | -6 080 | -11 530 | 0 | 0 | -42.930 | 0 |
| 7023100 | CU3(PO4)2 | -7 810 | 36.850 | 0 | 36.900 | -42.930 | 18.140 |
| 7023101 | CU3(PO4)2.3W | -10 747 | 35 120 | -2 630 | -3.420 | -10.737 | -1.440 |
| 6023104 | CUSO4 | -8 097 | -3 010 | 2 960 | 2.135 | 3.200 | 8 960 |
| 6023105 | CHALCANTHITE | -3 297 | 2 640 | 0 | 0 | 21.861 | 38.690 |
| 2023102 | DIOPTASE | 15 581 | -6 500 | -5 350 | 0 | -12 871 | 17.480 |
| 3023100 | CUPRICFERRIT | -19 901 | -7 030 | 0 | -7.060 | -13.402 | 4 360 |
| 4195000 | ZNCL2 | -0 402 | 10 000 | 10 810 | 9.820 | -13.402 | 0 |
| 5055000 | SMITHSONITE | -3 142 | 10 260 | 0 | 0 | 7.402 | 0 |
| 5055001 | ZNCO3. 1H2O | -5 048 | -12 450 | -12 260 | -12 480 | 7.402 | 0 |
| 2095000 | ZN(OH)2 (A) | -4 798 | -12 200 | 0 | 0 | 7.402 | 0 |
| 2095001 | ZN(OH)2 (C) | -4 340 | -11 750 | -11.320 | -11 890 | 7 402 | 0 |
| 2095002 | ZN(OH)2 (B) | -4 508 | -11 710 | -11.190 | -11.440 | 7 402 | 0 |
| 2095003 | ZN(OH)2 (G) | -4 098 | -11 500 | -10.950 | -11 620 | 4 667 | 0 |
| 2095004 | ZN(OH)2 (E) | -10 533 | -15 200 | 0 | 0 | 16.735 | 0 |
| 4195001 | ZN2(OH)3CL | -21 705 | -38 508 | 0 | 0 | -3 200 | 0 |
| 4195002 | ZN5(OH)8CL2 | -10 700 | 7 500 | 0 | 0 | 11.603 | 0 |
| 6095000 | ZN2(OH)2SO4 | -16 797 | 28 400 | 0 | 0 | -14 813 | -5 510 |
| 6095001 | ZN4(OH)6S04 | -18 256 | -11 310 | -11 570 | -11.860 | 7 402 | 0 |
| 519S000 | ZNNO3)2.6H2O | -3 390 | -11 140 | -10.990 | -11.540 | 7 402 | 21 860 |
| 2095005 | ZNO/ACF(VF) | 3 738 | 19 070 | 0 | 0 | -13 802 | 62 000 |
| 6095002 | ZN2NISP412 | -12 832 | 32 040 | 0 | 0 | -42.521 | 0 |
| 7095000 | ZN3(PO4)1.4W | -10 404 | 930 | 0 | 0 | -3 330 | 18 270 |
| 6735000 | ZNS1O3 | -4 509 | 15 130 | 10 150 | 0 | 0 | 0 |
| H0250H0 | WILLEUITE | | | | | | |

| ID | Mineral | | | | | |
|---|---|---|---|---|---|---|
| 5080000 | CERRUSITE | -2.389 | 13.130 | 13.440 | 12.830 | -15.519 | -4.860 |
| 2050000 | MASSICOT | -7.526 | -12.910 | -12.790 | | 5.284 | 16.780 |
| 2060001 | LITHARGE | -7.436 | -12.720 | -12.640 | -13.070 | 5.284 | 16.380 |
| 2060002 | PBO. 3H2O | -7.696 | -12.980 | 0 | 0 | 5.284 | 0 |
| 5060001 | PB2OCO3 | -9.734 | .500 | .780 | 0 | -10.234 | 11.460 |
| 6060000 | LARNAKITE | -7.154 | .280 | 6.300 | 0 | -7.434 | 6.440 |
| 6060001 | PB*2S04 | -12.550 | -10.400 | 0 | 0 | -2.150 | 20.750 |
| 6060002 | PB403S04 | -10.965 | -22.100 | 0 | 34.510 | 3.135 | 35.070 |
| 7060001 | CLPYROMRPH | 3.624 | 84.430 | 0 | 0 | -80.806 | 0 |
| 7060002 | HXYPYROMORPH | -7.080 | 62.790 | 0 | 0 | -70.670 | 0 |
| 5060002 | PB3O2CO3 | -15.970 | -11.020 | 0 | 0 | -4.950 | 26.430 |
| 7060005 | TSUMEBITE | -4.739 | .790 | 0 | 0 | -14.529 | 0 |
| 82600N0 | PBS1O3 | -6.099 | -7.320 | -6.120 | -7.640 | 1.221 | 9.260 |
| 8060000 | PM2S1O4 | -13.254 | -19.760 | -19.220 | -20.050 | 6.506 | 26.000 |
| 6060003 | ANGLESITE | -4.929 | 7.790 | 7.870 | 0 | -12.719 | -2.150 |
| 2060004 | PB1G)12 (C) | -2.866 | -8.150 | 0 | -13.630 | 5.284 | 13.990 |
| 4160003 | LAURIONITE | -5.475 | .623 | -.177 | 0 | -4.832 | 0 |
| 4160004 "B210M)3CL | -8.361 | -8.793 | 0 | 0 | 4.432 | 0 |
| 5060000 | HYDCCROUSITE | 8.293 | 17.140 | 0 | -27.100 | -25.753 | 0 |
| 2060005 | PB2O(OH)12 | -15.631 | -26.200 | 0 | 0 | 10.549 | 0 |
| 5060004 | PB41OM15SO4 | -17.935 | -21.600 | 0 | 0 | 3.135 | 0 |
| 5023101 | MALACHITE | -1.031 | -5.180 | 0 | 3.940 | -6.271 | 15.610 |
| 5023102 | AZURITE | -2.289 | 16.320 | 0 | 0 | -19.000 | 23.770 |
| 4293000N | 2M1B0212 | -12.533 | -8.200 | 0 | 0 | -4.341 | 0 |
| 52600N0 | PB1B02I2 | -14.070 | -7.010 | 0 | 0 | -6.160 | 5.800 |
| 7047C31 | MNMPO4(C) | 1.008 | 25.400 | 0 | 0 | -24.392 | 0 |
| 7060006 | PBMPO4 | -3.180 | 23.900 | 0 | 0 | -27.000 | 0 |
| 7060007 | PBCIPPM12 | -4.075 | 44.500 | 0 | 0 | -48.075 | 0 |
| 2015000 | LIME | -21.935 | -32.797 | 0 | 0 | 10.862 | 46.265 |
| 2015001 | PORTLANDITE | -11.813 | -22.675 | 0 | 0 | 10.662 | 30.690 |
| 2046001 | PERICLASE | -11.186 | -21.510 | 0 | 0 | 10.321 | 36.135 |
| 3016001 | MAG-FERPITE | -8.154 | -16.765 | 0 | 0 | 24.919 | 66.639 |
| 8215002 | WOLLASTOMITE | -6.197 | -12.996 | 0 | 0 | 6.799 | 19.496 |
| 8215003 | P-WOLLSTOMIT | -7.047 | -13.846 | 0 | 0 | 6.799 | 21.068 |
| 8015001 | CA-OLIVINE | -19.980 | -37.649 | 0 | 0 | 17.660 | 54.695 |
| 8015002 | LARNITE | -21.481 | -39.141 | 0 | 0 | 17.660 | 57.238 |
| 6015007 | CA3S1U5 | -45.345 | -77.867 | 0 | 0 | 28.522 | 106.335 |
| 6015003 | MONTICELLITE | -13.149 | -20.272 | 0 | 0 | 17.173 | 49.421 |
| 8015005 | AKERMINITE | -23.551 | -47.472 | 0 | 0 | 23.921 | 76.445 |
| 8015004 | MERWINITE | -43.730 | -68.543 | 0 | 0 | 34.783 | 107.111 |
| 3028102 | LEPIOMCOOCIT | 5.927 | -1.371 | 0 | 0 | 7.298 | 0 |

NORMAL TERMINATION OF MINTEO

# END

# FILMED

5-85

# DTIC